Ministry of Environment and Food of Denmark
Environmental Protection Agency

Environmental and health screening profiles of phosphorous flame retardants

A LOUS follow-up project

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Preface

Alternatives to halogenated flame retardants are to a large extent based on phosphorus chemistry. The Danish EPA has identified a lack of data on environmental and health effects of many of the phosphorous flame retardants and a lack of uniform data that can be used by companies who want to substitute phosphorous flame retardants for halogenated flame retardants.

This project compiles information about marketed phosphorous flame retardants, evaluates and modifies a screening tool for assessing flame retardants and other substances, and presents human health and environmental hazard screening profiles for a selected number of flame retardants in order to help companies to identify potential alternatives to halogenated flame retardants.

This revised version has been prepared in October 2016 in response to comments received from industry and Clean Productin Action to the report. The revision mainly concerns the description of the GreenScreen® method as well as the description of diethylphosphinate, aluminium salt (CAS No. 225789-38-8) and the description of polyphosphonate and phosphonate oligomers (both with CAS No. 68664-06-2).

Steering group
The project has been followed by a steering group consisting of:

- Toke Winther, Danish EPA (Chairman)
- Jesper Gruvmark, Danish EPA
- Carsten Lassen, COWI
- Jesper Kjølholt, COWI

Working group
The project has been carried out from July 2015 to November 2015 by a working group consisting of Carsten Lassen (Project Manager), Marlies Warming, Anna Brinch, Julie Zwicky Burkal, Jesper Kjølholt and Sonja Hagen Mikkelsen, COWI A/S, Denmark.

Summary and conclusion

Alternatives to halogenated flame retardants are to a large extent based on phosphorus chemistry. The Danish EPA has identified a lack of data on environmental and health effects of many of the phosphorous flame retardants and a lack of uniform data that can be used by companies who want to substitute phosphorous flame retardants for halogenated flame retardants.

The aim of this project has been to identify phosphorous flame retardants and develop screening level substance hazard profiles, to be used for substitution consideration in a European REACH context by companies using flame retardants.

The screening hazard profiles have been prepared based on a modified version of a method for hazard assessment of chemicals known as GreenScreen® for Safer Chemicals (GreenScreen®). GreenScreen® was developed based on the US EPA "Design for the Environment" (DfE) programme, as well as other international and national frameworks including Global Harmonized System of Classification and Labelling of Chemicals (GHS) and the European Union's Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH). It consists of a hazard profiling part and a "benchmarking" part aimed to assess the relevance of a substance for consideration in a substitution context. For some effect categories the GreenScreen® hazard criteria are different from the criteria used in the DfE assessments. For the purpose of the current project, the method was reviewed and modified taking into account a European regulatory context and the focus in this project on chemical hazard assessment in relation to consumer products.

Long list of phosphorous flame retardants
A gross list of 88 phosphorous flame retardant substances has been compiled based on literature and information on websites of manufacturers of flame retardants organised in the two trade associations EFRA (European Flame Retardants Association) and Pinfa (Phosphorus, Inorganic and Nitrogen Flame Retardants Association). Of these, approximately 50-60 different flame retardants substances are manufactured today. The two organisations represent all major manufacturers of flame retardants in Europe and the USA, and the list thereby is considered to include the main phosphorous flame retardants produced in this part of the world. The number cannot be estimated exactly as many of the flame retardants have proprietary (confidential) CAS numbers and chemical names. The substances are used in various flame retardant products (in combination with other constituents and other flame retardant substances), and the number of different flame retardant products is considerably higher than the number of substances.

The long list includes information on CAS No, chemical name, structural and general formula, phosphorous content, product and manufacturer names, and the tonnage registered under REACH.

Review and modification of the GreenScreen® methodology
A critical review of the GreenScreen® methodology was performed to evaluate its applicability for hazard assessment related to consumers and the environment in a European regulatory context. Based on this, the method was modified prior to use for hazard profiling in this report.

The EU applicability of the methodology has been addressed by critically reviewing the following main elements:

- i) the data sources to be used and their relative importance,
- ii) the hazard classification criteria, and
- iii) the alternatives assessment strategy and criteria for benchmarking of the substances.

The review revealed that the GreenScreen® methodology was developed using an internationally oriented approach with REACH and CLP/GHS criteria and guidance documents as key data for classifying the substances and recommends internationally recognized data sources. Thus, the approach was found to be in line also with Danish EPA and ECHA guidance documents for hazard identification. Consequently, the suggested adaptations of the hazard profiling part of the method are relatively minor and mainly concern the priority of some data sources, small adjustments of a few hazard classification limits, e.g. those for bioaccumulation, and omission of physical hazards from the hazard profiles (considered irrelevant in the consumer product context in the current project). A pilot test using the modified methodology was conducted on two substances, one previously assessed by the US EPA and one new substance. The modified screening profile of the substance previously evaluated by the US EPA differed from the earlier assessment only with regard to endocrine activity (not scored by US EPA) and bioaccumulation (score changed from "high" to "moderate" due to proposed changes in criteria limits for this endpoint).

As regards the benchmarking part of the GreenScreen® methodology, the only modification introduced is omission of criteria related to physical hazards, in consequence of the omission of these parameters in the hazard profiling part.

Selection of phosphorous flame retardants for screening

Besides a re-evaluation using the modified methodology of 23 flame retardant substances screened as part of the US EPA DfE programme, five flame retardants were selected for screening in this study. The five flame retardants were selected from the long list based on the following criteria: 1) The substance is already to some extent used as an alternative to halogenated flame retardants or marketed specifically as such; 2) the substance meets the applicable fire safety requirement for major applications of some halogenated flame retardants; 3) the substance is registered under REACH, or significant environmental and health data are available otherwise; and 4) the substance is not classified as a CMR substance in accordance with the CLP Regulation (Regulation (EC) No 1272/2008). The re-evaluation with the modified methodology was based on data provided by the US EPA DfE programme and no additional data has been used.

Applicability and screening profiles of manufactured phosphorous flame retardants

Using the modified screening method, screening profiles and overall hazard scores have been developed for 28 substances as summarised in Table 1. In the case where no modifications are suggested and where there are differences between the GreenScreen® hazard criteria and the criteria in the US EPA DfE programme, the criteria from the Dfe programme have been used. The table furthermore includes screening profiles for some of the main halogenated flame retardants (more US EPA profiles shown in Appendix 1). Please note that the brominated flame retardants are typically used together with antimony trioxide, which has a harmonised classification as carcinogenic.

Besides the screening profiles, for each of the identified manufactured phosphorous flame retardants, information on the applicability of the flame retardants has been reviewed and summarised. The summarised information includes:

- Applicability for each of the substrates as indicated by Pinfa's Product Selector[1];
- Substrates (type of plastics, paint, textiles, etc.) as indicated by manufacturers;
- End applications (automotive, building sector, etc.) as indicated by manufacturers;
- Interaction with substrate (additive, reactive);
- Availability (recently introduced, widely applied, main flame retardant for the applications, etc.) to the extent data are available from manufacturers or the literature.
- Flame retardancy: Various information on the ability of the flame retardants in meeting different fire safety standards for relevant substrates as indicated in the literature, technical data sheets, etc. The description is built on the information readily available for each flame retardant.
- Halogen-containing flame retardants for the same application to the extent it is described in the literature or from the manufacturers' product selectors.

The review shows that phosphorous flame retardants are available for the major applications of halogenated flame retardants. The indications of applicability are mainly provided on an overall level. The list may be used to identify relevant alternative flame retardants. However, more specific information on applicability and price should be obtained from the listed manufacturers in a concrete substitution context.

Discussion of the applicability of the modified GreenScreen method

The hazard profiling methodology is assessed to be applicable to human health and environmental hazard profiling of chemical substances in a European context, not only for substances belonging to the group of flame retardants addressed in this project, but for hazard profiling of chemicals of possible concern in general. Flame retardant systems often consist of a mixture of several flame retardants and it should be noted that an assessment of a flame retardant system would include an assessment of each of the components. As an example the brominated flame retardants would often be used in combination with antimony trioxide so this substance should be included in the screening as well. The current GreenScreen Guidance does not provide any decision logic for deriving a single benchmark score for the mixture, but a practical approach would be to use the benchmark score for the component with the lowest score (i.e. highest hazard) as decisive for the total score of the mixture. Benchmark scoring is possible even if data are not available for all hazard endpoints. E.g. data on sensitization are not necessary in order to score at the second highest benchmark level (BM3), however scoring at the highest level (BM4) is only permissible for substances where data for all endpoints exist. If the aim of the assessment is to identify possible alternatives to a given chemical, it is recommended to start with a rough assessment based on the harmonised classification or the selfclassification in the ECHA C&L inventory before starting to prepare a full hazard profile for a substance.

It should be emphasized that hazard profiling using this screening tool must be performed by persons with solid professional capability and experience within toxicology/human health assessment and environmental assessment in order to obtain reliable, balanced substance profiles, not least when assessing substances with incomplete data sets or with conflicting data for the same effect parameter. Additionally, in some cases it may be necessary to generate/estimate data by use of QSAR modelling tools, which can require special expertise. For the substances assessed in this study, no new QSAR modelling has been carried out, however available QSAR-based data (e.g. from the Danish (Q)SAR Database) have been used, where relevant.

[1] http://pinfa.org/index.php/product-selector

As regards the benchmarking part of the methodology, i.e. an assessment of the relevance of substances in a substitution context, the exercise of scoring the 28 phosphorous substances revealed that the majority of the substances ended up in the second-lowest overall hazard category (2) and only three substances obtained a better score (i.e. 3 or 4). The highest scores are for ammonium polyphosphate, poly[phosphonate-co-carbonate] and phosphinic acid, aluminium salt (3:1), whereas the aryl phosphates in general scores low (1). Thus, the differentiation between the substances appears to be too low to be operational in a substitution situation. This outcome was, at least to some extent, caused by a "gap" between two benchmark criteria levels (BM1 and BM2) in the GreenScreen® method, resulting in some substances obtaining a benchmark score that do not appear to fully reflect their hazard potential (i.e. a too high score). Hence, an additional benchmark level ("BM1½") could in principle be relevant to introduce for future occasions. However, neither BM1½ nor BM2 are probably substances being very relevant to consider as possible alternatives in the long.

Finally, it should be noted that in a substitution decision-making situation, the hazard profile of a substance cannot stand alone but must be complemented by exposure considerations for relevant use scenarios. This could e.g. result in placing more weight on some endpoints than others for a specific use scenario. E.g. in many consumer product contexts (i.e. product where possible release will take over time), "acute toxicity" will not be relevant because acute concentrations are not likely to occur in reality and, hence, this endpoint could either be omitted or be given lower weight than chronic endpoints.

Furthermore, the mobility of the substance in the polymer matrix should be taken into account. Reactive flame retardants, are chemically bound to the polymer matrix, and are consequently expected to have lower mobility and volatility than additive flame retardants and would result in lower exposure levels especially in the use phase of the product life cycle. Polymeric flame retardants would likewise be expected to have lower mobility and volatility, resulting in lower exposure levels during the use phase.

TABLE 1
HAZARD PROFILES AND OVERALL HAZARD SCORES BASED ON THE MODIFIED GREENSCREEN METHOD FOR SELECTED HALOGENATED AND PHOSPHOROUS FLAME RETARDANTS.

Chemical name	CAS No.	Group I Human					Group II and II* Human									Ecotox		Fate		Overall hazard score
		C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
								single	repeat*	single	repeat*									
Organophosphorous compounds																				
9,10-Dihydro-9-oxa-10-phosphaphenanthren-10-oxide (DOPO) *[Re]	35948-25-5	M	L	L	M	DG	L	DG	L	DG	M	M	DG	L	M	L	M	H	VL	2
N,N-bis-(2-hydroxylethyl) aminomethane phosphonic acid diethyl ester	2781-11-5	M	M	L	L	DG	L	DG	M	DG	M	M	DG	L	L	M	L	H	L	2
Poly(m-phenylene methylphosphonate) *[Re]	63747-58-0	L	L	M	M	H	L	DG	M	DG	M	L	DG	L	L	H	H	VH	H	1
Phosphonate oligomers (reactive) *[Re]	68664-06-2	M	L	L	L	DG	L	L	L	M	M	L	DG	M	M	L	H	VH	H	2
Poly[phosphonate-co-carbonate]	77226-90-5	L	L	L	L	L	L	L	L	L	L	L	DG	L	L	L	L	VH	L	3
Phosphoric acid, mixed esters with [1,1'-bisphenyl-4,4'-diol] and phenol	1003300-73-9	M	L	L	L	DG	L	DG	L	DG	L	L	DG	L	L	H	H	H	L	2
Oligomerisk phosphonate polyol *[Re]	363626-50-0	M	M	L	M	DG	L	L	L	M	M	L	DG	L	L	L	M	M	L	2
Organophosphates (phosphate esters) – Aryl phosphates																				
Triphenyl phosphate	115-86-6	M	L	L	L	H	L	DG	H	DG	L	L	DG	L	L	VH	VH	L	L	1
Tricresyl phosphate	1330-78-5	L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1
Cresyl diphenyl phosphate	26444-49-5	L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1
Phosphoric acid, bis(methylphenyl) phenyl ester	26446-73-1	L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1
Resorcinol bis-diphenyl phosphate	57583-54-7 / 125997-21-9	M	L	L	M	H	L	DG	M	DG	M	L	DG	L	L	VH	VH	M	H	1
Bisphenol A bis(diphenyl phosphate)	5945-33-5 / 181028-79-5	M	L	DG	L	DG	L	DG	L	DG	L	L	DG	L	L	L	L	H	M	2
Organophosphates (phosphate esters) – Alkyl phosphates																				

Chemical name	CAS No.	Group I Human					Group II and II* Human									Ecotox		Fate		Overall hazard score
		C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
								single	repeat*	single	repeat*									
Oligomeric ethyl ethylene phosphate	184538-58-7	L	M	L	L	DG	L	DG	L	DG	M	L	DG	L	M	L	L	VH	L	2
Organophosphates (phosphate esters) – Aryl alkyl phosphates																				
Isopropyl phenyl phosphate	68937-41-7	M	L	H	M	DG	L	DG	H	H	H	L	DG	L	L	VH	VH	M	VH	1
Tris (p-t-butylphenyl) phosphate	78-33-1	M	L	M	L	DG	L	DG	H	DG	M	M	DG	M	L	VH	VH	M	H	2
Phenol, isobutylenated, phosphate (3:1); Reaction mass of 4-tert-butylphenyl diphenyl phosphate and bis(4-tertbutylphenyl) phenyl phosphate and triphenyl phosphate **	68937-40-6	DG	L	L	L	DG	L	DG	M	M	M	L	DG	M	M	VH	VH	L	M	2
Melamine-derived and other organic phosphates (not being esters)																				
Melamine pyrophosphate	15541-60-3	M	M	L	L	DG	L	DG	M	L	L	L	DG	L	L	L	L	H	L	2
Diphosphoric acid, compd. with piperazine , and substituted amine phosphate	66034-17-1 and confid.	M	M	M	M	DG	H	DG	M	DG	DG	L	M	L	M	M	L	H	L	2
Melamine phosphate **	41583-09-9	M	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	DG	L	L	VH	VL	2
Ethylenediamine-o-phosphate **	14852-17-6	L	L	L	M	DG		DG	M	DG	DG	H	H	VH	L	M	H	VL	VL	2
Inorganic phosphorous compounds																				
Ammonium polyphosphate	68333-79-9	L	L	L	L	L	L	L	L	L	L	L	DG	L	L	L	L	(VH)	L	4
Red phosphorus	7723-14-0	L	M	L	L	DG	L	L	L	L	L	L	DG	M	M	L	L	H	L	2
Phosphinic acid, aluminium salt (3:1)**	7784-22-7	DG	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	M	M	M	(VH)	L	3
Other phosphorous and non-categorised substances																				
Diethylphosphinate, aluminium	225789-38-8	L	L	L	M	DG	L	M	M	DG	M	L	DG	VL	L	M	M	H	L	2
Confidential halogen-free flame retardant, Emerald Innovation™ NH-1	Confidential	M	L	M	L	H	H	DG	H	DG	M	M	DG	M	M	VH	VH	M	H	1
Fyrol™ HF-5 **	Confidential	M	M	L	M	H	L	DG	M	DG	M	L	DG	L	M	VH	VH	VH	M	1
6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide **	848820-98-4	DG	DG	DG	DG	DG	L	DG	DG	DG	DG	L	DG	H	DG	M	M	H	L	2

Chemical name	CAS No.	Group I Human					Group II and II* Human									Ecotox		Fate		Overall hazard score
		C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
								single	repeat*	single	repeat*									
Halogenated flame retardants (examples)																				
Decabrominated diphenyl ether (decaBDE)	1163-19-5	**M**	**L**	**L**	**H**	**H**	**L**	DG	**M**	DG	L	**L**	DG	**L**	**L**	L	L	**VH**	H	1
Tetrabromobisphenol A (TBBPA) *[Re] (also used additive)	79-94-7	**M**	**L**	**L**	**M**	**H**	**L**	DG	**L**	**L**	**L**	**L**	DG	**L**	**M**	**VH**	**H**	**H**	**M**	1
Hexabromocyclododecane (HBCDD)	25637-99-4	M	**L**	**M**	**H**	**H**	**L**	DG	**M**	M	M	**L**	DG	**L**	**L**	**VH**	**VH**	**H**	**VH**	1
Tris (1-chloro-2-propyl) phosphate (TCCP)	13674-84-5	M	**L**	**H**	**H**	M	**L**	DG	**M**	M	**M**	**L**	DG	**L**	**L**	**M**	**M**	**H**	**L**	1

*[Re]: Reactive flame retardants; **: Hazard profiles prepared as part of this study, whereas the remainder are based on US EPA (2014 a, 2014 b, 2015)

C = Carcinogenicity
M = Mutagenicity
R = Reproductive toxicity
D = Developmental toxicity
E = Endocrine activity
AT = Acute mammalian toxicity

ST = Systemic toxicity
N = Neurotoxicity
SnS = Skin sensitization
SnR = Respiratory sensitization
IrS = Skin irritation
IrE = Eye irritation
AA = Acute aquatic toxicity

N = Neurotoxicity

AA = Acute aquatic toxicity
CA = Chronic aquatic toxicity
P = Persistence
B = Bioaccumulation

VL Very Low hazard
L Low hazard
M Moderate hazard
H High hazard
VH Very High hazard
( ) Indicate specific assessments for inorganic substances for which the standard scoring criteria are not valid.

DG: Data Gap (on a white background) means that due to lack of data no hazard score has been assigned
Bold font: hazard score is based on measured/empirical data
Normal font: the hazard score is based on estimated/predicted values (e.g. QSAR) or on read-across and/or other expert judgement

Sammenfatning og konklusion

Alternativer til halogenerede flammehæmmere er i vid udstrækning baseret på fosforkemi. Miljøstyrelsen har identificeret en mangel på data vedrørende miljø- og sundhedsmæssige effekter af mange af de fosforbaserede flammehæmmere samt en mangel på ensartede data, der kan bruges af virksomheder, der ønsker at erstatte halogenerede flammehæmmere med fosforbaserede flammehæmmere.

Formålet med dette projekt er at identificere fosforbaserede flammehæmmere og udvikle fareprofiler på screeningsniveau for de enkelte stoffer, som i europæisk REACH sammenhæng skal kunne bruges af virksomheder der anvender flammehæmmere.

Farescreeningsprofilerne er blevet udviklet på baggrund a en modificeret metode, der er kendt som GreenScreen® for Safer Chemicals (GreenScreen®). GreenScreen® er baseret på den amerikanske miljøstyrelses "Design for the Environment" (DfE) program samt på internationale og nationale reguleringer, herunder Global Harmonized System of Classification and Labelling of Chemicals (GHS) og EU's Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH). Metoden anvendes til at opstille fareprofiler og tildele Benchmark Scores, som medvirker til at vurdere et givent kemisk stof i en substitutionskontekst. For nogle effektkategorier adskiller GreenScreen® kriterierne sig fra kriterierne anvendt i DfE vurderingerne. Metodens anvendelighed som beslutningsværktøj, der kan bruges af virksomheder i deres bestræbelser på at erstatte farlige stoffer i produkter, er blevet evalueret i en europæisk lovgivningsmæssig kontekst og på baggrund af dette projekts fokus på farevurdering af kemikalier i relation til forbrugerprodukter.

Bruttolisten af fosforbaserede flammehæmmere
En bruttoliste på 88 fosforbaserede flammehæmmere er blevet udarbejdet på grundlag af en litteraturgennemgang og information fra hjemmesider af producenter af flammehæmmere, som er medlemmer i brancheforeningerne EFRA (European Flame Retardants Association) og Pinfa (Phosphorus, Inorganic and Nitrogen Flame Retardants Association).

På bruttolisten er der 50-60 forskellige flammehæmmere, som fremstilles i dag. Tallet kan ikke angives præcist, for mange af flammehæmmerne har fortrolige CAS-numre og fortrolige kemiske navne. De to organisationer repræsenterer alle større producenter af flammehæmmere i Europa og USA, og listen vurderes dermed at omfatte de væsentligste fosforbaserede flammehæmmere, som produceres i denne del af verden. Stofferne anvendes i forskellige flammehæmmende produkter (i kombination med andre komponenter og andre flammehæmmende stoffer), og antallet af flammehæmmende produkter er betydeligt højere end antallet af stoffer. Bruttolisten indeholder oplysninger om CAS-nr., kemisk navn, strukturformel, sumformel, fosforindhold, produktnavne og producentnavne, og den registrerede tonnage i henhold til REACH.

Gennemgang og modificering af GreenScreen® metodologien
En kritisk gennemgang af GreenScreen® metoden er blevet udført i dette projekt med henblik på vurdering af metodens anvendelighed til farevurdering relateret til forbrugerprodukter og miljø i en europæisk kontekst. Metoden blev således modificeret inden den blev anvendt til farescreening i nærværende rapport.

Anvendeligheden af metoden er blevet behandlet ved at gennemgå følgende hovedelementer:

- i) hvilke datakilder, der skal anvendes til screeningen, og deres relative betydning,
- ii) kriterier for fareklassificeringen, og
- iii) vurderingsstrategien for alternativer og kriterier for "benchmarking" af stofferne.

Gennemgangen viste, at GreenScreen® metoden er blevet udviklet med en international tilgang, hvori REACH og CLP/GHS kriterier og vejledninger indgår som centrale datakilder til vurderingen af stofferne. Derudover anbefales brugen af internationalt anerkendte datakilder i metoden. Tilgangen er derfor også i overensstemmelse med Miljøstyrelsens og ECHAs vejledninger om fareidentifikation. De foreslåede tilpasninger af farescreeningen i metoden er derfor relativt små. Den største tilpasning gælder prioriteringen af nogle datakilder, små justeringer af enkelte grænseværdier i scoringskriterierne, f.eks. for bioakkumulering, og udeladelse af fysiske farer fra screeningsprofilerne (anses som irrelevant i forbrugerkontekst i nærværende projekt). Den modificerede metode er blevet testet på to stoffer, ét som tidligere er blevet vurderet af den amerikanske miljøstyrelse og ét nyt stof. Screeningsprofilen af det stof, som er blevet vurderet før, afveg kun på hormonforstyrrende aktivitet (som ikke vurderes af den amerikanske miljøstyrelse) og bioakkumulering (score blev ændret fra "high" til "moderate" baseret på foreslået ændring af grænseværdierne i kriteriet for bioakkumulering) fra den tidligere vurdering.

Med hensyn til Benchmark-delen af GreenScreen® metoden, er udeladelse af kriterier vedrørende fysiske farer den eneste ændring. Denne ændring følger af udeladelsen af disse parametre i farescreeningen.

Udvælgelse af fosforbaserede flammehæmmere til screening

Ud over en revurdering med den modificerede metode af 23 flammehæmmende stoffer, som blev screenet som en del af den amerikanske miljøstyrelses DfE program, blev fem flammehæmmere udvalgt til farescreening i denne undersøgelse. De fem flammehæmmere blev udvalgt fra bruttolisten ud fra følgende kriterier: 1) Stoffet anvendes allerede i et vist omfang som alternativ til halogenerede flammehæmmere eller bliver markedsført specifikt som sådan; 2) stoffet opfylder de foreskrevne brandkrav til hovedanvendelser af nogle af de halogenerede flammehæmmere; 3) stoffet er registreret i henhold til REACH, eller væsentlige miljø- og sundhedsmæssige data er tilgængelige på anden måde; og 4) stoffet er ikke klassificeret som et CMR-stof i henhold til CLP-forordningen (forordning (EF) nr. 1272/2008). Revurderingen med den modificerede metode var baseret på data fra den amerikanske miljøstyrelses DfE program, og der er ikke benyttet yderligere data.

Anvendelsesområde og screening profiler af fosforbaserede flammehæmmere

Screeningsprofiler og overordnede fare scores er blevet udviklet til 28 stoffer med den modificerede screeningsmetode som vist i Tabel 1. I de tilfælde, hvor ingen modificeringer er foreslået, og hvor der er forskelle mellem GreenScreen® kriterierne og de kriterier, som anvendes i DfE programmet, er kriterierne fra Dfe programmet brugt. Tabellen viser derudover screeningsprofiler for nogle af de mest anvendte halogenerede flammehæmmere (flere profiler fra Dfe programmet er vist i bilag 1).

For hver af de identificerede fosforbaserede flammehæmmere er oplysninger om anvendeligheden gennemgået og sammenfattet. Disse oplysninger omfatter:

- Anvendelighed til forskellige substrater, som de er angivet i Pinfa's Product Selector[2];
- Substrater (type plast, maling, tekstiler mm) som angivet af producenterne;
- Slutanvendelser (bilindustrien, byggesektoren, etc.), som angivet af producenterne;
- Interaktion med substratet (additiv, reaktiv);
- Tilgængelighed (for nyligt indført, udbredt anvendelse, vigtigste flammehæmmere for bestemte anvendelser) i det omfang som data er tilgængelige fra producenterne eller litteratur;
- Flammehæmning: Oplysninger om hvorvidt flammehæmmerne møder de forskellige brandsikkerhedskrav for relevante substrater som angivet i litteraturen, i tekniske datablade mv.; Beskrivelsen bygger på de umiddelbart tilgængelige oplysninger.
- Halogenerede flammehæmmere for samme anvendelse i det omfang, som det er beskrevet i litteraturen eller fra producenternes produktvælgere.

Gennemgangen viser, at fosforbaserede flammehæmmere er tilgængelige for de fleste anvendelser af halogenerede flammehæmmere, men informationer om anvendelighed er hovedsageligt på et overordnet niveau. Listen kan bruges til at identificere relevante flammehæmmere. I en konkret substitutionssituation skal yderligere oplysninger om anvendelsesområde og pris indhentes fra de anførte producenter.

Diskussion af anvendeligheden af den modificerede GreenScreen-metode

Screeningsmetoden vurderes at kunne anvendes til sundheds- og miljøfarescreening af kemiske stoffer i en europæisk sammenhæng. Dette gælder ikke kun stoffer, som tilhører gruppen af flammehæmmere, men også andre mulige problematiske stoffer. Flammehæmmersystemer består ofte af en blanding af forskellige flammehæmmere, og det skal bemærkes, at en screening af et flammehæmmersystem vil bestå af en screening af alle komponenter. Eksempelvis anvendes bromerede flammehæmmere i kombination med antimon trioxid, så dette stof vil også skulle indgå i screeningen. Gældende retningslinjer for GreenScreen® oplyser ikke, hvordan man får en benchmark score for en blanding, men en praktisk tilgang ville være at bruge benchmark scoren for den komponent, som får den laveste score (dvs. med den højeste risiko), som udslagsgivende for den samlede score af blandingen. Det er muligt at udarbejde en benchmark score, selv om der ikke er tilgængelige data for alle endpoints. Eksempelvis vil data vedrørende sensibilisering ikke være nødvendige for at kunne opnå en benchmark score på det næsthøjeste niveau (BM3), men det er kun muligt at opnå den højeste score (BM4), hvis der findes data for alle endpoints. Hvis formålet med vurderingen er, at identificere mulige alternativer for et givent stof, anbefales det, at begynde med en overordnet benchmark vurdering baseret på den harmoniserede klassificering eller selvklassificeringen angivet i REACH C&L inventory, før der udarbejdes et fuldstændigt fareprofil for et stof.

Det skal understreges, at farescreening med dette screeningsværktøj skal udføres af personer med solid faglig baggrund og erfaring inden for toksikologi/sundheds- og miljøvurdering for at opnå pålidelige stofprofiler. Dette er især vigtigt ved vurderingen af stoffer med ufuldstændigt datasæt eller ved modstridende data for samme effekt-parameter. Derudover kan det i nogle tilfælde være nødvendigt at generere data ved hjælp af QSAR modellerings-værktøjer, hvilket kræver særlig ekspertise. For de stoffer, der er vurderet i denne undersøgelse, er der ikke udarbejdet nye QSAR modelleringer, men tilgængelige QSAR-baserede data (f.eks. fra den danske (Q)SAR Database) er anvendt, hvor det har været relevant.

[2] http://pinfa.org/index.php/product-selector

Med hensyn til tildeling af de overordnede fare scores, som afspejler en vurdering af, hvor relevant et stof er med henblik på substitution, viser scoringen af de 28 fosforbaserede flammehæmmere, at de fleste stoffer endte i en overordnet fare kategori 2. Kun tre stoffer opnåede en bedre score (dvs. 3 eller 4). Den højeste score blev opnået for ammonium polyfosfat, poly[fosfonat-co-carbonat] og fosfinsyre, aluminium salt (3:1), hvor i mod arylfosfaterne generelt fik en lav score (1). Differentieringen mellem stofferne lader derfor til at være for lav for at kunne anvendes operationelt i en substitutionssituation. Dette skyldes til dels et "gab" mellem to af benchmark niveauerne (BM1 og BM2) i GreenScreen® metoden, som resulterer i, at nogle stoffer får en benchmark score, som ikke helt reflekterer deres farepotentiale (dvs. de får for høj en score). Det kunne i princippet - for fremtidige anvendelser af metoden -være relevant at indføre et ekstra benchmark niveau (BM1½). Det er dog også således, at det på langt sigt næppe vil være relevant at overveje, hverken stoffer som opnår BM1½ eller BM2 som mulige alternativer.

Endelig skal det bemærkes, at farescreeningen af et stof ikke kan stå alene i en beslutningsproces om substitution, men skal suppleres med eksponeringsovervejelser i relevante anvendelsesscenarier. Screeningsresultatet kunne f.eks. påvirkes af, at der lægges mere vægt på nogle effektparametre, som er særlig relevante for et bestemt anvendelsesscenarie. I sammenhæng med mange forbrugerprodukter vil "akut toksicitet" eksempelvis ikke være en relevant parameter, fordi koncentrationer, som er så høje, at de ville kunne medføre akutte effekter, aldrig vil forekomme i forbrugerprodukter. Derfor kunne denne parameter enten udelades eller i det mindste tildeles lavere vægt end de kroniske parametre.

Derudover bør der tages hensyn til mobilitet af stoffet i polymermatricen. Reaktive flammehæmmere er bundet i polymermatricen, og må derfor forventes at have en lavere mobilitet og flygtighed end additive flammehæmmere. Lavere mobilitet og flygtighed vil resultere i lavere eksponeringsniveauer, især i produktets brugsfase. Polymere flammehæmmere vil ligeledes forventes at have lavere mobilitet og flygtighed, hvilket resulterer i lavere eksponeringsniveauer i brugsfasen.

TABEL 1
FAREPROFILER OG OVERORDNEDE FARE SCORES BASEREDE PÅ DEN MODIFICEREDE GREENSCREEN METODE FOR UDVALGTE HALOGENEREDE OG FOSFORBASEREDE FLAMMEHÆMMERE.

Kemisk navn	CAS Nr.	Gruppe I Human					Gruppe II og II* Human									Økotoksicitet		Skæbne		Over-ordnet fare score
		C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
								enkelt	gen-tagen*	enkelt	gentag-en*									
Organofosforforbindelser																				
9,10-Dihydro-9-oxa-10-fosfophenanthren-10-oxid (DOPO) *[Re]	35948-25-5	M	L	L	M	DG	L	DG	L	DG	M	M	DG	L	M	L	M	H	VL	2
N,N-bis-(2-hydroxylethyl) aminomethan fosfonsyre diethylester	2781-11-5	M	M	L	L	DG	L	DG	M	DG	M	M	DG	L	L	M	L	H	L	2
Poly(m-phenylen methylfosfonat) **	63747-58-0	L	L	M	M	H	L	DG	M	DG	M	L	DG	L	L	H	H	VH	H	1
Fosfonat oligomerer (reaktive) [Re]	68664-06-2	M	L	L	L	DG	L	L	L	M	M	L	DG	M	M	L	H	VH	H	2
Poly[fosfonat-co-karbonat] **	77226-90-5	L	L	L	L	L	L	L	L	L	L	L	DG	L	L	L	L	VH	L	3
Fosforsyre, blandende estre med [1,1'-bisphenyl-4,4'-diol] og fenol	1003300-73-9	M	L	L	L	DG	L	DG	L	DG	L	L	DG	L	L	H	H	H	L	2
Oligomeric fosfonatepolyol *[Re]	363626-50-0	M	M	L	M	DG	L	L	L	M	M	L	DG	L	L	L	M	M	L	2
Organofosfater (fosfat ester) – Aryl fosfater																				
Triphenylfosfat	115-86-6	M	L	L	L	H	L	DG	H	DG	L	L	DG	L	L	VH	VH	L	L	1
Tricresylfosfat	1330-78-5	L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1
Cresyl diphenylfosfat	26444-49-5	L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1
Fosforsyre, bis(methylphenyl) phenyl ester	26446-73-1	L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1
Resorcinol bis-diphenylfosfat **	57583-54-7 / 125997-21-9	M	L	L	M	H	L	DG	M	DG	M	L	DG	L	L	VH	VH	M	H	1
Bisphenol A bis(diphenylfosfat)	5945-33-5 / 181028-79-5	M	L	DG	L	DG	L	DG	L	DG	L	L	DG	L	L	L	L	H	M	2
Organfosfater (fosfat ester)– Alkyl fosfater																				
Oligomeric ethyl ethylenfosfat	184538-58-7	L	M	L	L	DG	L	DG	L	DG	M	L	DG	L	M	L	L	VH	L	2
Organfosfater (fosfat ester) – Aryl alkyl fosfater																				

Kemisk navn	CAS Nr.	Gruppe I Human					Gruppe II og II* Human									Økotoksicitet		Skæbne		Overordnet fare score
		C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
								enkelt	gentagen*	enkelt	gentagen*									
Isopropyl phenylfosfate	68937-41-7	M	L	H	M	DG	L	DG	H	H	H	L	DG	L	L	VH	VH	M	VH	1
Tris (p-t-butylphenyl)fosfate	78-33-1	M	L	M	L	DG	L	DG	H	DG	M	M	DG	M	L	VH	VH	M	H	2
Phenol, isobutylenated, fosfat (3:1); Reaktionsprodukt af 4-tert-butylphenyl diphenylfosfat og bis(4-tertbutylphenyl) phenylfosfat og triphenylfosfat	68937-40-6	DG	L	L	L	DG	L	DG	M	M	M	L	DG	M	M	VH	VH	L	M	2
Melamin-afledte og andre organiske fosfater (ikke ester)																				
Melamin pyrofosfat	15541-60-3	M	M	L	L	DG	L	DG	M	L	L	L	DG	L	L	L	L	H	L	2
Difosforsyre, forbindelser med piperazin , og substitueret aminfosfat	66034-17-1 and confid.	M	M	M	M	DG	H	DG	M	DG	DG	L	M	L	M	M	L	H	L	2
Melaminfosfat	41583-09-9	M	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	DG	L	L	VH	VL	2
Ethylendiamin-o-fosfat	14852-17-6	L	L	L	M	DG		DG	M	DG	DG	H	H	VH	L	M	H	VL	VL	2
Uorganiske fosfatforbindelser																				
Ammonium polyfosfat **	68333-79-9	L	L	L	L	L	L	L	L	L	L	L	DG	L	L	L	L	(VH)	L	4
Rød fosfor	7723-14-0	L	M	L	L	DG	L	L	L	L	L	L	DG	M	M	L	L	H	L	2
Fosfinsyre, aluminium salt (3:1)	7784-22-7	DG	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	M	M	M	(VH)	L	3
Andre fosforforbindelser og ikke kategoriserede forbindelser																				
Diethylfosfinat, aluminium salt	225789-38-8	L	L	L	M	DG	L	M	M	DG	M	L	DG	VL	L	M	M	H	L	2
Fortrolig halogen-fri flammehæmmer, Emerald Innovation™ NH-1	Confid.	M	L	M	L	H	H	DG	H	DG	M	M	DG	M	M	VH	VH	M	H	1
Fyrol™ HF-5 **	Confid.	M	M	L	M	H	L	DG	M	DG	M	L	DG	L	M	VH	VH	VH	M	1
6H-Dibenz[c,e][1,2]oxafosforin-6-propansyre, butyl ester, 6-oxid	848820-98-4	DG	DG	DG	DG	DG	L	DG	DG	DG	DG	L	DG	H	DG	M	M	H	L	2

Kemisk navn	CAS Nr.	Gruppe I Human					Gruppe II og II* Human									Økotoksicitet		Skæbne		Overordnet fare score
		C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
								enkelt	gentagen*	enkelt	gentagen*									
Halogenerede flammehæmmere (eksempler)																				
Decabromineret diphenyl ether (decaBDE)	1163-19-5	**M**	**L**	**L**	**H**	**H**	**L**	DG	**M**	DG	L	**L**	DG	**L**	**L**	L	L	**VH**	H	1
Tetrabromobisphenol A (TBBPA) *[Re] (også brugt additivt)	79-94-7	**M**	**L**	**L**	**M**	**H**	**L**	DG	**L**	**L**	**L**	**L**	DG	**L**	**M**	**VH**	**H**	**H**	**M**	1
Hexabromocyclododecan (HBCDD)	25637-99-4	M	**L**	**M**	**H**	**H**	**L**	DG	**M**	M	M	**L**	DG	**L**	**L**	**VH**	**VH**	**H**	**VH**	1
Tris (1-chloro-2-propyl) fosfat (TCCP)	13674-84-5	M	**L**	**H**	**H**	M	**L**	DG	**M**	M	**M**	**L**	DG	**L**	**L**	**M**	**M**	**H**	**L**	1

*[Re]: Reative flammehæmmere; **: Fareprofiler udarbejdet i denne undersøgelse; de øvrige er baseret på US EPA (2014a, 2014 b; 2015).

C = Kræftfremkaldende M = Mutagenicitet R = Reproduktionstoksicitet D = Udviklingstoksicitet E = Hormonforstyrrende aktivitet AT = Akut toksicitet for pattedyr	ST = Systemisk toksicitet N = Neurotoksicitet SnS = Hudsensibilisering SNR = Respiratorisk sensibilisering IRS = Hudirritation Ire = Øjenirritation AA = Akut toksicitet for vandmiljøet N = Neurotoksicitet	AA = Akut toksicitet for vandmiljøet CA = Kronisk toksicitet for vandmiljøet P = Persistens B = Bioakkumulering	**VL** Meget lav fare **L** Lav fare **M** Moderat fare **H** Høj fare **VH** Meget høj fare **( )** Angiver specifikke vurderinger for uorganiske stoffer, hvor standard scoring kriterierne ikke er gyldige.	**DG:** Data mangel (på hvid baggrund) betyder, at ingen fare score kunne blivce tildelt på grund af manglende data. **Fed skrift**: Fare score er baseret på målte/ empiriske data. **Normal skrift**: Fare score er baseret på estimerede data (f.eks. QSAR) eller på analogislutninger og/eller ekspertvurderinger

1. Introduction

1.1 Background

The Danish Environmental Protection Agency (Danish EPA) has during the period 2012 to 2015 prepared surveys of 40 substances and substance groups on the agency's List of Undesirable Substances (LOUS). Two LOUS surveys - of brominated flame retardants (Lassen et al., 2014) and the chlorinated flame retardant TCCP (Larsen et al., 2014), respectively - identified a lack of information on relevant alternatives to these halogenated flame retardants.

A number of tools to assess chemical alternatives exist. One of the tools is the GreenScreen® for Safer Chemicals developed by the American NGO "Clean Production Action", which is based in part on an assessment method originally developed by the US Environmental Protection Agency (US EPA) as part of the programme "Design for the Environment" (DfE). The method is a transparent tool for evaluating and differentiating among chemicals based on their human health and environmental hazards. Screening profiles exist for a large number of phosphorous flame retardants from US EPA's DfE programme. It should be noted that the GreenScreen® criteria for some effects are different from the criteria used in the DfE programme and, hence, hazard profiles developed by the use of the GreenScreen method may be slightly different that the profiles developed in the DfE programme.

1.2 Objectives

The project has the following objectives:

- to present data on the technical and fire safety properties of marketed phosphorous flame retardants
- to evaluate and modify the GreenScreen® method with respect to compatibility in a European context in order to develop a screening tool, which can be used by companies who want to replace halogenated flame retardants
- to develop screening profiles for selected flame retardants according to the modified GreenScreen® method.

1.3 Activities

The following activities have been conducted within the project:

1.3.1 Compilation of the 'Long list of phosphorous flame retardants'

Based on literature search comprising information from manufacturers, reports on flame retardants, papers and other relevant literature, a long list of identified phosphorous flame retardants has been compiled. The list presents an overview of potentially relevant flame retardants (see chapter 2). Twenty eight substances from this list where selected according to criteria described in chapter for evaluation according to the modified GreenScreen® method.

1.3.2 Evaluation and modification of the GreenScreen® method

The GreenScreen® method is a tool for evaluating and differentiating among chemicals based on their human health and environmental hazards. The method has been developed in the USA, therefore its applicability in a European context has been analysed.

Chapter 0 presents the original GreenScreen® method and suggest modifications according to a European context. Furthermore, the applicability of the method on flame retardants, which are potential alternatives to halogenated flame retardants, is tested on two examples substances.

1.3.3 Technical descriptions and development of hazard profiles for selected flame retardants

Hazard profiles based on the modified GreenScreen® method were developed for 28 marketed phosphorous flame retardants which have been selected from the long list of identified flame retardants and which may be used as alternatives for halogenated flame retardants. For the sake of comparison, screening profiles for four of the main halogenated flame retardants are also included.

In the case where no modifications are suggested and where there are differences between the GreenScreen® hazard criteria and the criteria in the US EPA DfE programme, the criteria from the Dfe programme have been used.

In combination with a technical description of the flame retardants, the hazard profiles provide companies with a quick overview of the properties of potential alternatives.

In the light of substitution, development of smoke and hazardous substances from flame retardants in case of fire, are also an important parameter. Available information on this topic is presented in chapter 5.

2. Long list of phosphorous flame retardants

A long list of identified phosphorous flame retardants has been developed and is shown in Table 1. The list consists of phosphorous flame retardants identified from the following data sources:

- Websites of manufacturers organised in the two trade associations EFRA (European Flame Retardants Association) and Pinfa (Phosphorus, Inorganic and Nitrogen Flame Retardants Association.
- Reports developed under the US EPA Design for the Environment Programme (US EPA, 2014a,b,c, 2015).
- The Non-Halogenated Flame Retardant Handbook (Morgan and Wilkie, 2014).
- Two papers listing relevant phosphorus flame retardants (Bergman et al., 2012; van der Veen and de Boer, 2012).
- Other relevant literature identified in the project (SFT, 2009, Lassen et al., 1999, Lassen et al., 2006; Kemi, 2004, 2005; Arcadis, 2011)

For flame retardants marketed today, the information in Table 2 is supplemented with further information in chapter 3 and Appendix 10.

Reference
For flame retardants manufactured today, the names of the flame retardant products and the manufacturers are indicated. Some of the flame retardant products may contain more flame retardant substances in combination. For other flame retardants, a reference to the literature where the flame retardant is listed is indicated.

Registered volume
For substances registered under REACH, the registered volume is indicated. For non-polymeric substances it gives an indication of the total market volume, but it should be noted that several of the flame retardants are polymers, which are consequently not registered under REACH. For non-polymeric flame retardants, which are indicated as pre-registered but not registered, the total market volume is below 100 t/y per manufacturer/importer of these substances (limit volume for the latest registration deadline).

Availability of US EPA environmental and health screening profile
Furthermore, the table indicates whether an environmental and health screening profile is available in the four reports from the US EPA Design for Environment (DfE) programs on alternatives to decaBDE, HBCDD brominated flame retardants in printed circuit boards (printed CB), or pentaBDE in polyurethane foams (PUR). Substances, for which profiles have been developed as part of the current study, are indicated by "this study".

Substrate
The substrate column indicates in which substrates (plastic types, textiles, mixtures) the flame retardants are applied as indicated in technical data sheets and other information at the websites of the manufacturers. This information is supplemented with information from the branch organisation PINFA's Product Selector and information from the literature in section 2.2.

TABLE 2
IDENTIFIED PHOSPHOROUS FLAME RETARDANTS

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufacturer **	REACH registered tonnage, t/year	H/E Profile***	Substrate (as indicated by manufacturers)	Reference*	Page
Organophosphorous compounds										
35948-25-5	252-813-7	9,10-Dihydro-9-oxa-10-phosphaphenanthren-10-oxide	DOPO	KCCS DO11 EVERFOS DOPO	Metadynea Everkem	1,000 – 10,000	Printed CB	ABS, flexible polyurethane, unsaturated polyester, epoxy resin, phenolics resin, coating (paint), textile (back coating)		56
2781-11-5	220-482-8	N,N-(bis)-hydroxyethyl-aminomethane phosphonic acid diethyl ester		Levagard 4090 N Fyrol™ 6	Lanxess ICL-IP Europe	Pre-registered	PUR	Rigid PUR foams, PF, EP and UP resins		58
63747-58-0	*613-366-7	Poly(m-phenylene methylphosphonate)	DEEP	Fyrol PMP	ICL-IP Europe	Pre-registered	Printed CB	Epoxy resins		60
68664-06-2	Not available	Phosphonate oligomers (reactive) (Mn <10,000)		NOFIA™ OL1001 NOFIA™ OL3001	FRX Polymers	Not reg/pre-reg	Deca	Unsaturated Polyesters, Epoxy, Polyurethane and Polyurea		62
68664-06-2	Not available	Polyphosphonates (Mn >10,000)		Nofia HM1100	FRX Polymers	Not reg/pre-reg	Deca	Unsaturated Polyesters, Epoxy, Polyurethane and Polyurea		255
77226-90-5	Not available	Poly[phosphonate-co-carbonate]		NOFIA™ CO3000 NOFIA™ CO6000	FRX Polymers	Not reg/pre-reg	Deca	HIPS/PPO, PC/ABS, Polycarbonate (PC)		64
1003300-73-9	Not available	Phosphoric acid, mixed esters with [1,1'-bisphenyl-4,4'-diol] and phenol	BPBP	ADK STAB FP-800	Adeka Palmarole	Not reg/pre-reg	Deca	Polycarbonates and polyesters, polymer blends such as PC/ABS and PC/HIPS.		66
363626-50-0	Not available	Oligomeric phosphonate polyol		Exolit® OP 560 Exolit® OP 550	Clariant	Not reg/pre-reg	PUR	Flexible polyurethane foams		68
20120-33-6	243-528-9	Dimethyl {3-[(hydroxymethyl)amino]-3-oxopropyl}phosphonate		EVERFOS CP	Everkem	100 – 1,000		Cotton textile		234
18755-43-6	242-555-3	Dimethyl propyl phosphonate	DMPP	Levagard DMPP	Lanxess	100 – 1,000		PIR/PUR rigid foams and thermosets		235

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
Not identified	Not identi-fied	Phosphine oxide diol and triol		Not identified		Not reg/pre-reg		PUR, PET, epoxy resins	SFT 2009	
78-38-6	201-111-9	Diethyl ethylphosphonate		Aflammit® PLF 822	THOR	Pre-registered		Rigid PUR and PIR foams, epoxy, unsaturated polyes-ters		236
15827-60-8	239-931-4	Diethylenetriamine-penta(methylene phos-phonic acid)				1,000 – 10,000			www.flam e-retardant-materi-al.com	
Organophosphates (phosphate esters)										
Aryl phosphates										
115-86-6	204-112-2	Triphenyl phosphate	TPHP	EVERFOS TP (TPP) Disflamoll TP Disflamoll TP liquid	Everkem Lanxess Lanxess	1,000 – 10,000	De-ca/PUR	PP, PE, PDM, PVC, HIPS, PC/ABS (alloys), PPO/HIPS (alloys), rigid and flexible polyurethane, TPU, Epoxy resin, phenolics resin, PC, textile (back coating), adhe-sive, rubbers, cellulose acetate, cellulose acetate butyrate and vinyl copoly-mer, PPE/HIPS		70
26967-76-0	248-147-1	Tri(4-isopropylphenyl) phosphate	TIBPP			Pre-registered			European Commis-sion 2011; KEMI 2005, 2009	
68937-40-6	273-065-8 / 700-990-0	Phenol, isobutylenated, phosphate (3:1); Reaction mass of 4-tert-		Reofos® LF-50; Disflamoll TP LXS	Green Lake Solutions Lanxess	1,000 – 10,000	This study	PVC, flexible polyurethanes, cellulosic resins, and syn-thetic rubber. Flame retard-		72

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
		butylphenyl diphenyl phosphate and bis(4-tertbutylphenyl) phenyl phosphate and triphenyl phosphate		51092				ant processing aid for engi-neering resins, such as modified PPO, polycar-bonate and polycarbonate blends		
1330-78-5	215-548-8	Tricresyl phosphate	TMPP	EVERFOS TCP Kronitex® TCP Disflamoll TKP Disflamoll TKP-P	Everkem Great lake solutions Lanxess Lanxess	1,000 – 10,000	PUR	PVC, PVC flexible, polyester, phenolics resin, Nitrocellulose lacquers and coatings and processing aid for natural and synthetic rubbers (NBR and SBR)		74
28109-00-4	248-849-8	Bis-(isopropylphenyl) phenyl phosphate				Pre-registered			European Commis-sion 2011	
28777-70-0	249-209-0	Tris-(tert-butylphenyl) phosphate	TBDP			Pre-registered			European Commis-sion 2011	
26444-49-5	247-693-8	Cresyl diphenyl phosphate	CDP	EVERFOS CDP Kronitex® CDP Disflamoll DPK	Everkem Great Lakes Solutions Lanxess	Pre-registered	PUR (in the assess-ment of 1330-78-5)	PVC, flexible polyurethane, epoxy resin, phenolics resin, PC/ABS blends, TPU compounds, PUR-foams (rigid and flexible) and rubbers		76
26446-73-1	247-708-8	Phosphoric acid, bis(methylphenyl) phenyl ester	MEHP; Meth-ylated triphenyl phosphates; Bis(methylphen yl) phenyl phosphate			Pre-registered	PUR (part of assess-ment of 1330-78-5)		US EPA 2015	76
57583-54-7 (sometimes 125997-21-9 is used inter-	260-830-6	Resorcinol bis-diphenyl phosphate	PBDPP	EVERFOS RDP Fyrolflex RDP AFLAMMIT® PLF 280	Everkem ICL-IP Europe THOR	1,000 – 10,000	Deca	EPDM, HIPS, PC/ABS (alloys), PPE/HIPS (alloys), TPU, epoxy resin, PC, modi-fied PPO,		79

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
chageably)										
5945-33-5 (sometimes 181028-79-5 is used inter-changeably)	425-220-8	Bisphenol A bis(diphenyl phosphate)	BPA-BDPP, BDP	ADK STAB FP-600 EVERFOS BP (BDP) Fyrolflex BDP	Adeka Pal-marole Everkem ICL-IP Europe	1,000-10,000	Deca	EPDM, HIPS, PC/ABS (alloys), PPE/HIPS (alloys), TPU, epoxy resin, PC, HIPS/PPO		81
25155-23-1	246-677-8	Trixylyl phosphate	TXP	EVERFOS TXP	Everkem	100 – 1,000		EPDM, PVC, PC/ABS (al-loys), rigid and flexible polyurethane, phenolics resin, Coating (paint), tex-tile (back coating), adhesive		237
65652-41-7	265-859-8	Bis-(tert-butylphenyl)phenyl phos-phate				Pre-registered		PVC	European Commis-sion 2011	
78-33-1	201-106-1	Tris-(p-tert-butylphenyl) phosphate	TBPP			Pre-registered	PUR		European Commis-sion 2011	87
1330-78-5, 78-32-0, 78-30-8 and 25155-23-1		Tri(m,p-cresyl) phosphate mixture		Lindol	ICL-IP Europe	1330-78-5: 1,000-10,000; 25155-23-1: 100-1,000 and 78-32-0 and 78-30-8: Pre-registered		PVC flexible, Cellulosic Plastic Composite		
Proprietary		Proprietary aromatic phosphate		Fyrolflex Sol-DP	ICL-IP Europe			HIPS/PPO, PC/PC ABS		
Proprietary		Proprietary halogen-free phosphorus ester		Fyrol A710	ICL-IP Europe			Flexible Polyurethane foams		

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
Proprietary		Proprietary		Emerald Innova-tion™ NH-1	Great Lake Solutions		PUR	Furniture and automotive flexible polyurethane foam applications.		106
Alkyl phosphates										
184538-58-7	*606-033-2	Oligomeric ethyl ethylene phosphate		Fyrol PNX Fyrol PNX-LE AFLAMMIT® PLF 140	ICL-IP Europe THOR	Pre-registered	PUR	Flexible and rigid polyure-thane foams, cellulosic plastic composite		83
78-40-0	201-114-5	Triethyl phosphate	TEP	Levagard TEP-Z	Lanxess	1,000 – 10,000		PIR / PUR rigid foams and thermosets		241
126-73-8	204-800-2	Tributyl phosphate	TNBP	Phosflex 4	ICL-IP Europe	1,000 – 10,000		PVC flexible, la-tex/adhesives, cellulosic plastic composite		242
1806-54-8	217-305-1	Trioctyl phosphate				Preregis-tered			KEMI 2005	
Not identified	Not identi-fied	Neoalkoxy tri (dioctyl phosphate) titanate							KEMI 2005	
78-42-2	201-116-6	Tris-(2-ethylhexyl) phos-phate	TEHP	Disflamoll TOF	Lanxess	1,000 – 10,000		Many types of polymers including PVC flexible, PUR, NBR, SBR and EPDM.		243
78-51-3	201-122-9	Tris(2-butoxyethyl) phos-phate	TBOEP	Phosflex T-BEP	ICL-IP Europe	1,000 – 10,000		Rubbers/elastomers, la-tex/adhesives		244
5301-78-0	*610-937-2	Pentaerythritol phoshate alcohol				Pre-registered			KEMI 2004	
Aryl alkyl phosphates										
68937-41-7	273-066-3	Isopropyl phenyl phos-phate		EVERFOS 1350 - 1950 series Reofos® 35 - 95 series	Everkem Great lake solutions	10,000-100,000	PUR	PVC, cellulosic resins, and synthetic rubber, EPDM, HIPS, PC/ABS (alloys), PPO/HIPS (alloys), rigid and flexible polyurethane, TPU, epoxyresin, phenolics		85

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
				Phosflex 31L Phosflex 41L	ICL-IP Europe			resin, PC, Coating (paint), textile (back coating), adhe-sive, rubbers.		
1241-94-7	214-987-2	Diphenyl (2-ethylhexyl) phosphate	DPO	Disflamoll DPO Phosflex 362	Lanxess ICL-IP Europe	1,000 – 10,000		PVC, thermoplastic polyure-thane, nitrile butadiene rubber, cellulose nitrate, cellulose acetate		245
28108-99-8	248-848-2	Diphenyl isopropyl phos-phate				Pre-registered			European Commis-sion 2011	
29761-21-5	249-828-6	Isodecyl diphenyl phos-phate		Phosflex 390	ICL-IP Europe	1,000 – 10,000		PVC flexible		246
56803-37-3	260-391-0	tert-butylphenyl diphenyl phosphate				Pre-registered			European Commis-sion 2011	
56803-37-3; 65652-41-7; 78-33-1 and 115-86-6	260-391-0, 265-859-8, 201-106-1, and 204-112-2	t-Butylated triphenyl phosphate mixture		Phosflex 71B	ICL-IP Europe	Substances are pre-registered individually, except 115-86-6: 1,000 – 10,000		HIPS/PPO, PC/PC ABS, PVC flexible		247
27460-02-2 and 142474-86-0		Linear alkyl diphenyl phosphate	Phosphoric acid, dodecyl diphenyl ester	Phosflex 418	ICL-IP Europe	27460-02-2 is Pre-registered		PVC flexible		
		Octyl diphenyl phosphate							KEMI 2005	
Organophosphites										

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
7789-79-9	232-190-8	Calcium phosphinate		Phoslite IP-C	Italmatch	Pre-registered		PC/ABS, polycarbonate PC, Rubbers/elastomers, PVC flexible	PINFA, 2015	
868-85-9	212-783-8	Dimethyl phosphonate	DMHP			1,000 – 10,000			SFT 2009	
756-79-9	Not identi-fied	Dimethyl methyl phos-phonate	DMMP			Not reg/pre-reg			Pinfa 2015	
Melamine-derived and other organic phosphates (not being esters)										
15541-60-3	239-590-1	Melamine pyrophosphate		EVERFLAM MPP-2 AFLAMMIT® PMN 370	Everkem THOR	Pre-registered	Deca, printed CB	Coating (paint), textile (back coating)		89
218768-84-4	*606-855-1	Melamine polyphosphate	MPP	Melapur® 200 range BUDIT 3141 AFLAMMIT® PMN 200	BASF Budenheim THOR	Not reg/pre-regiistered				248
20208-95-1	243-601-5	Melamine polyphosphate		EVERFLAM MPP-1	Everkem	Pre-registered		Polyester, PA		249
41583-09-9	255-449-7	Melamine phosphate		Melapur MP Budit 312 Melagard MP MPT11 AFLAMMIT® PMN 185	BASF Budenheim Italmatch Metadynea Austria THOR	1,000 – 10,000		Thermoplastics, polyolefins, elastomers, engineering resins, paints, intumescent fire retardant coating		91
1271168-40-1	Not availa-ble	Melamine-poly(aluminium phosphate)		Safire® 200	Floridienne Chimie s.a. (patent belongs to Catena additives)	Not reg/pre-reg		PA, Nylon, PBT, PE, PP, PS, HIPS, PPE		250
1271172-98-5	Not availa-	Melamine-poly(zinc phos-		Safire® 400		Not reg/pre-		EVA, PA, Nylon, PBT, PE,		251

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
	ble	phate)				reg		PUR, PVC flexible, TPE and TPV		
Not identified	Not identi-fied	Melamine-poly(magnesium phos-phate)		Safire® 600				PBT PA, Nylon		252
Not identified	Not identi-fied	Melamine ortophosphate		BUDIT 310	Budenheim					
94031-26-2	Not availa-ble	1,3,5-Triazine-2,4,6-triaminephosphate	Flame retard-ant P	PPP111	Metadynea Austria GmbH	Not reg/pre-reg		Intumescent flame retard-ant systems		253
66034-17-1	457-330-7	Diphosphoric acid, compd. with piperazine		ADK STAB FP-2100J ADK STAB FP-2200	Adeka Pal-marole	10 – 100	Deca			93
Inorganic phosphorous compounds										
68333-79-9	269-789-9	Ammonium polyphos-phate		BUDIT 3123 - 3178 series FR CROS 484 FR CROS C30 FR CROS C60 Exolit® AP series EVERFLAM APP AFLAMMIT® PCI 202 Preniphor EPFR-series	Budenheim Clariant Everkem Thor Presafer	10,000 - 100,000	PUR	Unsaturated polyester resin, acrylic resins, epoxy or phenolics. PP, PE, PP copolymers and PP blends, Rigid and flexible polyure-thane, TPU, epoxy resin, coating (paint)		95
68333-79-9 and 14728-39-9	269-789-9 and not identified	Polyphosphoric acids, ammonium salts	APP			CAS No 14728-39-9 is not pre-	PUR		European Commis-sion 2011;	See 95

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
						registered, See above for CAS No 68333-79-9			Stuer-Lauridsen et al. 2000; KemI 2004, 2005, 2009; UK HSE 2012; EFRA 2012	
		Based on ammonium polyphosphate		Phos-Chek ® LC95W Solution Phos-Chek ® LC95W FT936 / Fire-Trol 936 FT934 / Fire-Trol 934 FT931 / Fire-Trol 931 Phos-Chek ® LC95A-F BUDIT® IS 3001 AFLAMMIT® PPN series	BK Giu-linibk-giulini GmbH Budenheim THOR					
7723-14-0	918-594-3	Red phosphorus		Red Phosphorus HB 801 Red Phosphorus PU 6580 Exolit® RP series MASTERET series	Clariant	1,000 – 10,000	Deca	Solid plastics, closed cell foams, polymer adhesives polyisocyanurate and polyu-rethane rigid foams plastics, polyurethanes, synthetic and natural rubber latex systems polyolefines articles,		98

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufacturer **	REACH registered tonnage, t/year	H/E Profile***	Substrate (as indicated by manufacturers)	Reference*	Page
					Italmatch			epoxy resins polypropylene articles and sometimes in PA.		
7722-76-1	231-764-5	Monoammonium phosphate				1,000,000-10,000,000			KEMI 2004	
7783-28-0	231-987-8	Diammonium phosphate		Phos-Chek 259-F	BK Giulinibk-giulini GmbH	1,000,000-10,000,000		Wildfire control		255
7722-76-1; 7783-28-0	231-764-5; 231-987-8	Monoammonium Phosphate, Diammonium Phosphate		PHOS-CHEK® MVP-F PHOS-CHEK® MVP-Fx	BK Giulinibk-giulini GmbH	1,000,000-10,000,000 (for the two substances, respectively)		Wildfire control		
7784-22-7	479-150-8	Phosphinic acid, aluminium salt (3:1)		Phoslite B-series	Italmatch	10-100		PBT, Polyamide (PA), Polypropylene (PP), Themoplastic elastomers, XPS foam, Plypropylene foam (PP), Rubbers/Elastomers, Other textile fibers, Epoxy Resins, Unsaturated polyesters, PVC flexible,Polypropylene (PP), TPU, PE/EVA	PINFA, 2015	177
Not identified	Not identified	Aluminium phosphates		FR CROS 134 P FR CROS 134 T	Budenheim			Aluminium phosphates		257
Other phosphorous and non-categorised substances										
14852-17-6	238-914-9	Ethylenediamine-o-phosphate	EDAP	EP11 Aflammit® PCO 123/234	Metadynea Austria THOR	0-10		Polyolefins and in most thermoset applications. self-intumescent		102

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
225789-38-8	*607-114-5	Diethylphosphinate, alu-minium salt		Exolit® OP series	Clariant	Pre-registered	Printed CB	High temperature polyam-ides , polyesters, reinforced polyamide (6 and 66)		104
4090-51-1	223-829-1	2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulphide		Exolit® 5060 PK	Clariant	100 – 1,000		Viscose fibres		258
1402947-09-4	Not availa-ble	Ammonium 6H-diben-zo[c,e][1,2]oxaphosphinin-6-olate 6-oxide		DXA 12	Metadynea Austria	Not reg/pre-reg				259
98165-92-5	Not availa-ble	Phosphoric acid, bis[3-[(diphenoxyphos-phinyl)oxy]phenyl] phenyl ester				Not reg/pre-reg			Ecolabel 2014.	
83029-72-5	Not availa-ble	phosphoric acid, bis(4-(1-(4-(diphenoxyphos-phinyl)oxy)phenyl)-1-methylethyl) phenyl ester							Ecolabel 2014.	
Proprietary		Proprietary (19.5%P, 17,5%N) New substance (REACh registered in Europe, TSCA listed in USA).		AFLAMMIT® PCO 700	THOR					
Proprietary		Proprietary (14%P, 37%N) New substance (REACh registered in Europe, TSCA listed in USA)		AFLAMMIT® PCO 800	THOR					
Proprietary		Proprietary (24%P)		AFLAMMIT® PCO 900 (ex TL 1260F) AFLAMMIT® PCO	THOR					

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
				960 (ex TL 1260)						
Not identified	Not identi-fied	Isopropylated phosphate ester (8,3%P)		AFLAMMIT® PLF 150	THOR			PVC, rubber and flexible PUR foams. Can also be used as a processing aid in PC and PPO (and their respective blends)		
Not identified	Not identi-fied	Cyclic phosphonate (19%P)		AFLAMMIT® PLF 710	THOR					
Proprietary		Substituted Amine Phos-phate Mixture					Deca		US EPA 2015	93
Proprietary		Proprietary Phosphorus Ester Blend		Fyrol™ HF-5	ICL-IP Europe		PUR			108
Proprietary		Proprietary non-halogen phosphorus ester		Fyrol HF-4	ICL-IP Europe			Flexible Polyurethane foams		
Proprietary		Proprietary phosphorus ester		Fyrol® HF-10	ICL-IP Europe			Flexible Polyurethane foams		
Proprietary		Proprietary mixture of phosphate esters		Fyrol® HF-5HP	ICL-IP Europe			Flexible Polyurethane foams		
Proprietary		Proprietary		Fyrol® HF-9	ICL-IP Europe			Flexible Polyurethane foams		
Proprietary		Oligomeric phosphate ester		Levagard® TP LXS 51078	Lanxess			Flexible PUfoams		
848820-98-4	805-659-5	6H-Dibenz[c,e][1,2]oxaphosph otin-6-propanoic acid, butyl ester, 6-oxide	DOPO-AC4	DOB11 Levagard TP LXS 51114	Metadynea Austria Lanxess	10 – 100		Polyesters, PUR and epoxy-systems		
36240-31-0	Not availa-ble	10-Hydroxy-9,10-dihydro-9-oxa-10-	DOPO-OX, DOPO-OH	DX 11	Metadynea Austria	Not reg/pre-reg		polyesters, epoxy-systems, polyolefines		

CAS No	EC No	Chemical name	Abbreviation, trivial name	FR product	Manufac-turer **	REACH registered tonnage, t/year	H/E Pro-file***	Substrate (as indicated by manufacturers)	Refer-ence*	Page
		phosphaphenanthrene-10-oxide								

* For manufactured flame retardants reference is made to the web-sites of the manufacturers.

** If no indication of manufacturer, no flame retardants with the substance manufactured by companies that are members of EFRA and Pinfa have been identified

*** Profile refers to available US EPA profiles. Deca = US EPA 2014a, PUR = US EPA 2015, Printed CB = US EPA 2014b (see reference list)

An asterix before the EC number indicates that the substance has no EC number, but be the pre-registration or registration has been given a list number in the EC format.

3. Modification of the GreenScreen® methodology

In this chapter, a general level description of the original GreenScreen® method for hazard profiling and benchmarking for chemical alternatives assessment is given and adaptations/modifications for possible use of the method in a European regulatory context are presented based on a critical review of the original method combined with pilot testing on two substances. However, the intention has not been to provide a detailed review of all aspects of the methodology or to elaborate a use manual, merely to provide a foundation for the reader to understand the subsequent hazard profiling and scoring of 28 phosphorous-based flame retardants considered to be possible alternatives to a number of undesired brominated flame retardants. For full details on the basics of the methodology reference is made to the original description of GreenScreen® (Clean Production Action, 2013).

3.1 The GreenScreen® methodology

The GreenScreen® method was developed by the American NGO "Clean Production Action" and was first made publically available in 2011. The current version is V1.2 (Clean Production Action, 2013). GreenScreen® is based in part on an assessment method, "Alternatives Assessment Criteria for Hazard Evaluation", which was originally developed by the US Environmental Protection Agency (US EPA) as part of the programme "Design for the Environment" (DfE) as "*a transparent tool for evaluating and differentiating among chemicals based on their human health and environmental hazards*". GreenScreen® was thus not specifically developed to assess flame retardants.

GreenScreen® is a systematic screening level approach to documenting and classifying human health and environmental hazards associated with chemicals. GreenScreen® can be used for identifying chemicals of high concern and safer alternatives. It is used to support product design and development, materials procurement, and as part of alternatives assessment based on internationally accepted classification criteria. A GreenScreen® assessment of a chemical results in a summary hazard profile, which can be used for risk assessment, and a so-called benchmark score, which can be used to assess the potential of the chemical when searching for safer alternatives. Benchmarks scores are determined by analysing specific combinations of hazard classifications using a set of benchmarking criteria defined by GreenScreen®, which reflect hazard concerns established by governments nationally and internationally. The simplified procedure of a GreenScreen® assessment is shown below.

FIGURE 1
OVERVIEW OF THE GREENSCREEN® HAZARD ASSESSMENT PROCEDURE *(REPRODUCED AND SIMPLIFIED FROM CLEAN PRODUCTION ACTION, 2013)*

Each relevant toxicological and environmental property of the chemical being evaluated is "translated" into a hazard level ("High", "Moderate", or "Low" and in some cases “very High” or “very Low”) by applying one or more hazard criteria used by national (American) regulatory bodies, the European Union (REACH/CLP) or international organisations (e.g. OECD, IARC etc.).

Human health hazards are divided into Group I and Group II endpoints, where Group I covers hazards that can lead to chronic or life-threatening effects or adverse impacts that are potentially induced at low doses and transferred between generations, i.e. carcinogenicity, mutagenicity, genotoxicity, reproductive toxicity, developmental and neurodevelopmental toxicity, and endocrine activity. Group I endpoints have three hazard levels (H, M, L). Group II and II* cover systemic toxicity endpoints, sensitisation and skin and eye irritation. Group II endpoints (acute toxicity, systemic toxicity, neurotoxicity, and skin and eye irritation) are evaluated based on single exposure and are assigned one of four hazard levels (vH, H, M, L) whereas the Group II* endpoints (including systemic toxicity and neurotoxicity) are evaluated based on repeated exposure and are assigned one of three hazard levels (H, M, L). Group II* endpoints also include sensitisation.

Ecotoxicity, environmental fate and physical hazards endpoints are assigned four hazard levels except for persistence (P) and bioaccumulation (B) which are assigned five levels also including the "Very Low" (vL) level. Identified, relevant environmental transformation products should be taken into account in the hazard assessment of a substance.

An example GreenScreen® Hazard Summary Table is shown in Table 2.

TABLE 2
EXAMPLE OF A GREENSCREEN® HAZARD SUMMARY TABLE

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeat*	single	repeat*										
DG	*L*	*L*	**M**	**M**	DG	*L*	*L*	**M**	**M**	**L**	**L**	**L**	**L**	*L*	*L*	*vH*	*M*	*L*	*L*

Abbreviations:

C = Carcinogenicity	SnR = Respiratory sensitization	SnS = Skin sensitization
M = Mutagenicity	IrS = Skin irritation	CA = Chronic aquatic toxicity
R = Reproductive Toxicity	IrE = Eye irritation	P = Persistence
D = Developmental Toxicity	AA = Acute aquatic toxicity	B = Bioaccumulation
E = Endocrine activity	ST = Systemic toxicity	Rx = Reactivity
AT = Acute mammalian Toxicity	N = Neurotoxicity	F = Flammability

An example of the criteria applied for the hazard profiling, which are based on classifications by various regulatory bodies or international organisations, is presented below by the original GreenScreen® set of criteria for carcinogenicity (Table 3).

TABLE 3
GREENSCREEN® HAZARD CRITERIA FOR CARCINOGENICITY

	Information	Information	List type	High	Moderate	Low
Carcinogenicity (C)	Data	GHS Criteria & Guidance		GHS Category 1A (Known) or 1B (Presumed) for any route of exposure	GHS Category 2 (Suspected) for any route of exposure	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
	A lists	EU CMR *1	Authoritative	Category 1 or 2	Category 3	
		EU CMR *2	Authoritative	Carc 1A or 1B	Carc 2	
		EU H-	Authoritative	H350 or H350i	H351	
		EU R-phrases	Authoritative	R45 or R49	R40	
		EU SVHC	Authoritative	Reason for inclusion: Carcinogenic		
		IARC	Authoritative	Group 1 or 2A	Group 2B	Group 4
		MAK	Authoritative	Carcinogenic Group 1 or 2	Carcinogenic Group 3, 4, or 5	
		NIOSH-C	Authoritative	Occupational Cancer		
		NTP-RoC	Authoritative	Known or Reasonably Anticipated		
		Prop 65	Authoritative	Known to the state to cause cancer		
		EPA-C (1986)	Authoritative	Group A, B1 or B2	Group C	Group E
		EPA-C (1996,	Authoritative	Known or Likely		Not Likely
	B lists	EPA-C(1986)	Authoritative	Group D		
		EPA-C (1999)	Authoritative	Suggestive Evidence, but not sufficient to assess human carcinogenic potential		
		EPA-C (2005)	Authoritative	Suggestive evidence of carcinogenic potential		
		IARC	Authoritative	Group 3		

*1 Classification according to (DSD) Council Directive 67/548/EEC

*2 Classification according to (CLP) Regulation (EC) No 1272/2008

Following the hazard profiling of a substance, an assessment of its potential for being a possible alternative to an existing substance can, when relevant, be carried out using a stepwise so-called benchmarking approach as illustrated in Table 4 below.

Normally, the data identified in the hazard profiling process and the resulting scores in the summary hazard table are used for this purpose but a very rough, first assessment can be made based on substance classifications alone. Such a rough assessment will primarily serve to rapidly exclude substances without potential as alternatives before spending resources on a more in-depth identification and evaluation of specific data.

TABLE 4
GREENSCREEN® BENCHMARKS *(BASED ON CLEAN PRODUCTION ACTION, 2013). CRITERIA MARKED WITH GREY ARE THOSE ORIGINAL GREENSCREEN® CRITERIA, WHICH ARE OMITTED IN THE PROPOSED MODIFIED METHODOLOGY (PHYSICAL HAZARDS).*

Benchmark 1 (Avoid – Chemical of high concern)
a. PBT = High P + High B + [very High T (Ecotoxicity, Group II Human or High T (Group I and II* Human)]
b. vPvB = very High P + very High B
c. vPT = very High P + [very High T (Ecotoxicity, Group II Human) or High T (Group I and II* Human)]
d. vBT = very High B + [very High T (Ecotoxicity, Group II Human) or High T (Group I and II* Human)]
e. High T (Group I Human)
Benchmark 2 (Use but search for safer substitutes)
a. Moderate P + Moderate B + Moderate T (Ecotoxicity, Group I, II and II* Human)
b. High P + Hígh B
c. High P + Moderate T (Ecotoxicity, Group I, II and II* Human)
d. High B + Moderate T (Ecotoxicity, Group I, II and II* Human)
e. Moderste T (Group I Human)
f. Very High T (Ecotoxicity or Group II Human) or High T (Group II* Human)
g. High Flammability or High Reactivity
Benchmark 3 (Use but still opportunity for improvement)
a. Moderate P or Moderate B
b. Moderate Ecotoxicity
c. Moderate T (Group II or II* Human)
d. Moderate Flammability or Moderate Reactivity
Benchmark 4 (Prefer – safer chamical)
Low P + Low B + Low T (Ecotoxicity, Group I, II and II* Human) + Low Physical Hazards (Flammability and Reactivity) + Low (additional ecotoxicity endpoints when available)

As demonstrated by the illustration, the Benchmark 1 hazard criteria align to a large extent with the definition of a substance of very high concern (SVHC) under REACH, and a chemical may be assigned this score based on one endpoint only or a combination of endpoints. As an example a substance classified under GHS/CLP in category 1 for carcinogenicity will be assigned the benchmark 1 score as well a substance fulfilling the PBT criteria. Benchmark scores 2 and 3 are assigned based on either an individual criterion or a combination of criteria and the evaluation of a minimum data set for chemicals not achieving Benchmark 1, and Benchmark 4 is assigned to chemicals based on data for all 18 hazard endpoints when the resulting hazard levels are all in the low category.

3.2 Adaptation of the methodology to a European context

A critical review of the GreenScreen® methodology was performed to evaluate its applicability for hazard assessment related to consumers and the environment in a European regulatory context.

This evaluation of the methodology has focussed on the hazard classification/scoring criteria, the required data and the recommended documentation sources to ensure that the methodology reflects the principles and criteria in the current European chemical regulation (REACH and CLP) and also meets the Danish EPA's requirements to hazard assessment of chemical substances in consumer product projects. Also the procedure and criteria for the subsequent benchmark scoring

for assessment of the potential of a chemical as an alternative to existing chemicals have been reviewed critically.

To address this, the methodology has been critically reviewed with regard to the following:

i) data collection,
ii) criteria for hazard profiling,
iii) benchmarking procedure,
iv) criteria for alternatives assessment

The reviewed elements of the methodology have been compared to the information sources and perceived validity of health and environmental data recommended by the Danish EPA and/or ECHA for hazard assessment of chemicals, and the classifications and specific hazard criteria applied in Denmark and/or the EU. Subsequently, relevant modifications or adaptations of the methodology to the European context have been made. The evaluation and suggestions for adaptations are described in the sub-sections below.

The suggested modifications to the methodology and criteria are relatively minor as the review process confirmed that the GreenScreen® method was developed using already to a significant extent an internationally oriented approach with REACH and CLP/GHS criteria and guidance as key data for classifying the substances, and considering and incorporating internationally recognised data sources, including those recommended or requested by ECHA and the Danish EPA, in addition to specific North American lists of data sources. The details will be presented in the following sections.

When applying the modified method in this report it has to be noted that, in the case where no modifications are sugested and where there are differences between the GreenScreen® hazard criteria and the criteria in the US EPA DfE programme, the criteria from the DfE programme have been used.

3.2.1 Evaluation and adaptation of data sources

The list of information sources included in the GreenScreen® methodology was reviewed and found to comprise many of the same sources (factual and bibliographic databases/portals, homepages, model tools) that are commonly used also in Denmark when performing hazard and risk assessments of chemicals in consumer products (and of chemical substances in general). GreenScreen for Safer Chemicals Version 1.2 Information Sources document is intended to provide support for performing GreenScreen Assessments but is not intended to serve as an exhaustive and ordered list of all information sources that should be used to perform a hazard assessment on a chemical.

However, some bias towards US information sources was noted and, additionally, a few data sources were considered to address issues at a too detailed level for a screening assessment. Based on these considerations, a few information sources are suggested to be omitted and a few new ones proposed to be included. Also, fee-based databases have generally been omitted. Further, the order of appearance of the data sources has been changed partly to reflect the "European view", partly to organise the information sources a bit more systematically, i.e. in the following three main categories:

1) Classification databases,
2) factual databases and homepages (i.e. including review reports) and
3) model tool homepages and databases.

In the adapted data source list, the following data sources are omitted from the GreenScreen® list of information sources (version 1.2):

- CHE database (database which summarises links between chemical contaminants and approximately 180 human diseases or conditions. Omitted as the relevant information is expected to be covered by other sources)
- GHS (Substituted with CLP criteria)
- EPA RED (No additional relevant information provided)
- UM-BBD (Not accessible)
- RTECS (fee-based)
- LOLI (fee-based)
- Ariel (fee-based)
- ISSCAN (this model is expected to be covered by other included models)

The following data sources are added to the adapted GreenScreen® list of information sources (version 1.2):

- CLP (Substitutes GHS criteria)
- CLP advisory list for self-classification (added, Danish QSAR predictions)
- Gestis (Substance database from the German Social Accident Insurance containing information about approx. 9400 substances)

The list of information sources for a screening assessment with proposed modifications for a European context is shown in Table 5. For practical reasons, entries targeting several information sources, e.g. database portals such as eChemPortal and Toxnet, have been split up to show the direct links to the most relevant databases comprised by the portal, which are not already covered by an individual entry, as this supports a more systematic data search. These entries have been given a greyish shading.

TABLE 5
LIST OF INFORMATION SOURCES FOR GREENSCREEN® ASSESSMENT, MODIFIED TO A EUROPEAN CONTEXT. GREY-SHADED ENTRIES UNDER A DATABASE PORTAL ARE THOSE CONSIDERED MOST RELEVANT, AND WHICH DO NOT HAVE AN INDIVIDUAL ENTRY ALREADY.

ID	Abbreviation	Information Type	Information Source	URL and/or Reference
1	CLP	CLP Classifications and Substance Data	European Chemicals Agency, ECHA	http://echa.europa.eu/information-on-chemicals/cl-inventory-database
2	CLP advisory list for self-classification	Database with QSAR predictions for classification	Danish Environmental Protection Agency	http://mst.dk/virksomhed-myndighed/kemikalier/stoflister-og-databaser/vejledende-liste-til-selvklassificering-af-farlige-stoffer/clp/
3	REACH	Database (substance registration dossiers)	European Chemicals Agency, ECHA	http://echa.europa.eu/information-on-chemicals/registered-substances
4	eChemPortal	Database Portal	The Organisation for Economic Co-operation and Development eChemPortal	http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

ID	Abbreviation	Information Type	Information Source	URL and/or Reference
	EnviChem	Database	SYKE, Data Bank of Environmental Properties of Chemicals	http://www.ymparisto.fi/en-US/Maps_and_statistics/Data_systems/Data_bank_of_Environmental_Properties_of(30591)
	OECD HPV	Database	Organisation for Economic Cooperation and Development (OECD) Existing Chemicals Database	http://webnet.oecd.org/hpv/ui/Default.aspx
	GSBL	Database	Joint Substance Data Pool of the German Federal Government and the German Federal States	http://en.gsbl.de/gsblweb30/main.do;jsessionid=B029017C653833915C6451110B0BCC6E
5	INCHEM	Database Portal	Chemical Safety Information from Intergovernmental Organizations (IPCS, WHO, CCOHS, IOMC)	http://www.inchem.org/
	CICADs	Database	Concise International Chemical Assessment Documents	http://www.inchem.org/pages/cicads.html
	EHC	Database	Environmental Health Criteria Monographs	http://www.inchem.org/pages/ehc.html
	IARC	Database	International Agency for Research on Cancer (IARC) Monographs on the Evaluation of carcinogenic Risks to Humans	http://monographs.iarc.fr/
	JECFA	Database	Joint Expert Committee on Food Additives (JECFA) - Monographs and Evaluations	http://www.inchem.org/pages/jecfa.html
	SIDS	Database	OECD Screening Information Data Set (SIDS) High Production Volume Chemicals	http://www.inchem.org/pages/sids.html
	UKPID	Database	UK Poison Information Documents	http://www.inchem.org/pages/ukpids.html

ID	Abbreviation	Information Type	Information Source	URL and/or Reference
6	IRIS	Database	US Environmental Protection Agency (EPA), National Center for Environmental Assessment, Integrated Risk Information System (IRIS) Database	http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showSubstanceList
7	NIOSH/OSHA	Pocket Guide/Database	NIOSH Pocket Guide	http://www.cdc.gov/niosh/npg/
8	TOXNET	Database Portal	The Toxicology Data Network	http://toxnet.nlm.nih.gov/index.html
	HSDB	Database	The Toxicology Data Network	http://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
	TOXLINE	Database	The Toxicology Data Network	http://toxnet.nlm.nih.gov/newtoxnet/toxline.htm
	DART	Database	The Toxicology Data Network	http://toxnet.nlm.nih.gov/newtoxnet/dart.htm
	GENE-TOX	Database	The Toxicology Data Network	http://toxnet.nlm.nih.gov/newtoxnet/genetox.htm
9	ACToR	Database Portal	Aggregated Computational Toxicology Resource	http://actor.epa.gov/actor/faces/ACToRHome.jsp;jsessionid=3EDA0C36597CBD1945389C18D05A7E4
10	ECOTOX	Database	The ECOTOXicology Database (US EPA)	http://cfpub.epa.gov/ecotox/
11	Gestis	Database	Institut für Arbeitsschutz der Deutschen Gesetzlichen Unfallversicherung (IFA)	http://gestis.itrust.de/nxt/gateway.dll/gestis_de/000000.xml?f=templates$fn=default.htm$3.0
12	Scorecard	Database	Scorecard Chemical Profiles	http://scorecard.goodguide.com/chemical---profiles/
13	PubChem	Database	PubChem	http://pubchem.ncbi.nlm.nih.gov/
14	ASTDR	Database	US Department of Health and Human Services, Agency for Toxic Substance & Disease Registry	http://www.atsdr.cdc.gov/az/a.html

ID	Abbreviation	Information Type	Information Source	URL and/or Reference
15	ToxRefDB	Database	US EPA Toxicity Reference Database (ToxRefDB), which captures thousands of in vivo animal toxicity studies on hundreds of chemicals.	http://www.epa.gov/comptox/toxrefdb/
16	FDA - ED	Database	US Food and Drug Administration (FDA) Endocrine Disruptor Knowledge Base (EDKB)	http://www.fda.gov/scienceresearch/bioinformaticstools/endocrinedisruptorknowledge-base/default.htm
17	CHIRP	Database	Japan National Institute of Technology and Evaluation (NITE) Chemical Risk Information Platform (CHRIP)	http://www.safe.nite.go.jp/english/db.html
18	PAN	Database	Pesticide Action Network Pesticide Database	http://www.pesticideinfo.org/Search_Chemicals.jsp
19	SIN List and SIN similarity tool	Database	ChemSec, the International Chemical Secretariat	http://sinlist.chemsec.org/
20	EPI Suite	Model tool	US EPA EPI (Estimation Programs Interface) Suite™	http://www.epa.gov/oppt/exposure/pubs/episuite.htm
21	PBT Profiler	Model tool	US EPA PBT Profiler	http://www.pbtprofiler.net/
22	(Q)SAR	Model tool	Danish (Q)SAR Database	http://qsar.food.dtu.dk/
23	OECD Toolbox	Model tool	The Organisation for Economic Co-operation and Development (OECD)	http://www.oecd.org/chemicalsafety/risk-assessment/theoecdqsartoolbox.htm
24	OncoLogic™	Model tool	US EPA, Sustainable Futures	http://www.epa.gov/oppt/sf/pubs/oncologic.htm

In addition to the above table with information sources, Appendix 3 contains the modified version of GreenScreen's so-called "Specified List", which is a table with a collection of lists with e.g. human health and environmental classifications of chemicals according to defined hazard criteria. The list indicates whether the individual lists originate from authoritative (reliable) sources (see definitions at start of the appendix) or are of a screening level type of information (lower degree of validation).

Finally, GreenScreen's "List Translator" (see Appendix 4) should be mentioned. This is based on the same classification lists as mentioned above, however here with a further sub-division into hazard classification parameters and categories to which benchmark scores are assigned. This simple benchmarking approach can be used for a first, rough assessment of a chemical as to whether it has any potential at all for being considered in an alternatives assessment, and thereby whether it is worthwhile to use the required efforts and resources to develop a full, documented hazard profile for the substance. No modifications of this list have been suggested.

3.2.2 Evaluation and adaptation of criteria for hazard profiling

Overall, GreenScreen's categories for hazard profiling are found to reflect well the classification categories used in REACH and CLP (GHS). The classification criteria in some other countries such as Canada and a number of signatories to the GHS system under United Nations as part of the GreenScreen® methodology were during this review found to be irrelevant for assessments in a European context and have therefore been deleted in the proposed adapted criteria table.

Further, physical hazard parameters such as flammability and reactivity, which are included in the profiling according to the GreenScreen® methodology, were also considered of marginal relevance in the current context focusing on protection of consumers and the environment. In the situations where exposure of consumers and/or the environment can occur, it was based on expert judgement assessed that the chemical substances will not be present in sufficient amounts and concentrations for such physical hazards to be expressed. They were therefore omitted from the hazard profiling and subsequent benchmarking procedures.

The same argument could in many cases also apply to other hazard endpoints, such as acute toxicity in Group II Human and acute ecotoxicity. It is, however, not considered justifiable to generalize in the same way for these endpoints as for the physical hazards and therefore these endpoints are suggested to be evaluated specifically on a case-by-case basis. In this report no modifications with regard to these hazard endpoints have been introduced.

Specific needs for adaptation of human health and environmental and hazard criteria in a European context are described in the following.

A table with the full set of adapted criteria and associated information sources is included as Appendix 2 to this report, while other tables comprising human health and environmental classification lists and their assigned scores for benchmarking (i.e. scoring for alternatives assessment) are included as Appendix 3 and Appendix 4, respectively. In order not to confuse the modified version with the original GreenScreen® method, “hazard profile” is used instead of “modified GreenScreen® profile” for the hazard profiles developed in this report.

Human health hazard criteria

The GreenScreen® health hazard criteria are largely based on GHS criteria which correspond to the criteria implemented with CLP. For some hazard classes the criteria however include more categories than those implemented with CLP. This is the case for acute mammalian toxicity and for skin and eye irritation where the GreenScreen® method includes category 5 for acute toxicity, category 3 for skin irritation, and category 2B for eye irritation, which are not included in CLP.

Furthermore, the GreenScreen® method has singled out neurotoxicity from the systemic toxicity/organ effects using US EPA Guidance to define applicable neurotoxic effects and otherwise weight of evidence-based criteria to categorise the effects. As neurotoxicity is a relevant endpoint for organophosphorus compounds, it is suggested to keep this endpoint as an individual hazard class in the modified approach.

In addition to the specific classification criteria, a number of authoritative lists and screening lists are included. Some of these lists are developed in the US at a federal or state level, such as the Prop 65 List (California Proposition 65) administered by the California EPA and including chemicals known to the state to cause cancer or reproductive toxicity. Evaluations not developed at a federal level such as Prop 65 are removed from the modified approach. In general, if applying data/entries from these lists, it is important to be aware that they may be developed with very different purposes and evidence behind the listing.

Endocrine activity/disruption does not have a specific classification category under the CLP/GHS Regulation. Substances demonstrating endocrine activity/disruption are therefore only classified if they fulfil the criteria for classification of other endpoints covered by the Regulation, e.g. effects on fertility or developmental effects, which result in a classification for reproductive toxicity.

The GreenScreen® method for identifying endocrine activity/disruption is therefore list-based with a number of screening lists and SVHC substances, which have been included in the REACH Candidate List based on endocrine activity (equivalent level of concern) as the only authoritative list. With regard to lists developed by the EU, the priority list of chemicals developed within the EU-Strategy for Endocrine Disruptors is included as a screening list. The Endocrine Active Substances Information System (EASIS) is under development to update the existing EU database hosted by Directorate General (DG) for Environment. This list is suggested to be added to the methodology when finalised. Under the modified method if a substance has not been included in any of the mentioned lists, but experimental data are available, the substance's endocrine activity potential is scored according to the criteria for the EU priority list based on the data levels as specified in the OECD Conceptual Framework for Testing and Assessment of Endocrine Disrupting Chemicals (see Appendix 2; ECETOC, 2009). If no experimental data are available, the endpoint is marked as a data gap (DG) corresponding to category 3b (no data available) of the EU priority list. Apart from these comments, the human health assessment part of the current GreenScreen® method is considered appropriate and is not modified.

The following specific adaptations of the list of health categories and information sources were made:

Data:

- GHS is substituted with CLP

Lists added:

- CLP classifications by industry are added as a B-list
- ADR (substitute for DOT)

"A Lists" removed:

- Other country-specific GHS implementations
- DOT
- Prop 65
- NTP-RoC (Considered covered by IARC)
- NTP OHAaT (includes currently very few substances)

"B Lists" removed:

- EPA AMT
- G&L
- Boyes-N
- OSPAR
- WHMIS
- DOT

Environmental hazard criteria

The GreenScreen® environmental hazard criteria comprise only a few hazard categories: Acute aquatic toxicity, chronic aquatic toxicity, persistence and bioaccumulation. The translation of classification categories (or data based ranges) into GreenScreen® hazard profile categories ("High" - "Moderate" – "Low", in some cases complemented by "Very High" and "Very Low") is found to be highly inspired by REACH and CLP/GHS hazard classification, either using the different levels of hazard categories or hazard phrases/statements or the numerical intervals of the hazard data un-

derlying the classifications. In particular for the persistence and bioaccumulation categories, the profiling categories are directly inspired by the PBT and vPvB criteria in REACH.

The following specific adaptations of the environmental categories were made:

- EU H-statements for acute and chronic aquatic toxicity: Missing categories have been added;
- EU R-phrases for acute and chronic aquatic toxicity: Small corrections and addition of missing categories;
- CLP classifications by industry regarding acute and chronic aquatic toxicity added as a B-list (non-authoritative info);
- Persistence in air: Half-life <2 days changed to be a combined moderate-low category;
- Categories of High and Moderate Bioaccumulation potential as represented by BCF changed from >1000-5000 and >500-1000, respectively, to >2000-5000 and >500-2000, to reflect more correctly the EU PBT and vPvB category delimitations;
- Low and Very Low bioaccumulation potential as reflected by Log Kow changed to include an interval for "Low" (>3.0 to 4.0) and reducing "Very Low" to Log Kow <3.
- Adaptations of sources of criteria: As above for health criteria sources. Additionally, DSL is suggested to be removed from the list of sources of environmental criteria.

Hazard profile presentation

The colour codes and symbols/abbreviations used by GreenScreen® for presenting the substance hazard profiles in the summary hazard tables are suggested to be modified slightly in the context of this report as they were found to be, albeit stringent, somewhat overloaded with information and also contained more information on this form than the US EPA summary hazard profiles to be reviewed. E.g. it was found that assessment and comments on data quality and validity could be more adequately addressed in an accompanying short text than on tabular form.

Hence, the summary tables in the current report (using the modified approach) apply the following colour codes, symbols and abbreviations for presentation of the substance hazard profiles:

TABLE 6
OVERVIEW OF COLOUR CODES, SYMBOLS AND ABBREVIATIONS USED IN THE CURRENT REPORT FOR PRESENTATION OF SUBSTANCE HAZARD PROFILES IN SUMMARY HAZARD TABLES.

Colour code or symbol	Explanation
VL	Very Low hazard
L	Low hazard
M	Moderate hazard
H	High hazard
VH	Very High hazard
DG	DG = Data Gap (on a white background) means that due to lack of data no hazard score has been assigned
Bold	**"Bold"** font means that the hazard score is based on measured/empirical data
Normal	"Normal" font mean that the hazard score is based on estimated/predicted values (e.g. QSAR) or on read-across and/or other expert judgement
( )	Parentheses are used to indicate specific assessments for inorganic substances, in particular of persistence for which the standard scoring criteria are not valid.

3.2.3 Evaluation and adaptation of benchmarking criteria and procedure

The procedure and criteria for benchmarking of substances in a substitution context is basically considered to be useful and applicable for a screening level assessment in its current form (see Table 4 for definition of BM levels). However, as explained in the preceding section, in a European context, the modified GreenScreen® methodology is anticipated only to be used to assess hazards of chemical substances to consumers and/or the environment.

The physical hazards (flammability and reactivity) included in the original GreenScreen® benchmarking criteria are considered to be of marginal relevance within the scope for the current project (see section 3.2.2). Flammability and reactivity are mainly of relevance in the application of the flame retardants for manufacture of flame retarded products and the hazard criteria for these parameters are therefore suggested to be omitted from the benchmarking procedure as applied here (Benchmark levels 2 (2.g), 3 (3.d) and 4).

We have found it less evident to make a similar general distinction between the endpoints in Group II Human and have therefore adopted the full set of endpoints as defined in the original procedure. In order not to confuse the modified version with the original GreenScreen® method, “overall hazard score” is used instead of “benchmark score” for the hazard profiles developed in this report.

3.3 Pilot test of the modified methodology

Two phosphorous substances were selected for testing the modified GreenScreen® methodology; one substance that has already been screened by the US EPA, CAS no. 115-86-6, triphenyl phosphate, and one "new", i.e. not previously screened, substance: CAS no. 68937-40-6, phenol, isobutylenated, phosphate.

3.3.1 Triphenyl phosphate, CAS No 115-86-6

The screening of triphenyl phosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives to the flame retardant decaBDE (US EPA, 2014a).

The comparison of the result – the summary hazard table – with the original hazard summary table by US EPA (US EPA 2014a) is shown in Table 7 and Table 8, respectively. The US EPA's presentation of the results slightly deviates from the original GreenScreen® summary table format and it was therefore found necessary to slightly adapt the presentation for the purpose of the current project. The US EPA does not include endocrine activity in the hazard comparison because of limited data for evaluation and lack of robust tools for modelling endocrine activity. Nonetheless, the US EPA lists studies on endocrine activity, if such data were available. In addition, the US EPA includes a category for repeated dose toxicity but not "systemic toxicity from single exposure" as it is the case in GreenScreen®. With regard to neurotoxicity the US EPA has one category whereas the GreenScreen® method differentiates between neurotoxicity from single and repeated exposure, respectively.

TABLE 7
US EPA SCREENING RESULT FOR TRIPHENYL PHOSPHATE (FORMAT SLIGHTLY MODIFIED TO FIT INTO CURRENT GREENSCREEN® FORMAT)

Group I Human					Group II and II* Human									Ecotox		Fate	
C	M	R	D	E[1]	AT	ST		N		SnS*	SnR*[3]	IrS	IrE	AA	CA	P	B
						single[2]	repeat*	single[2]	repeat*								
M	L	L	L		L	DG	H	DG	L	L		VL	L	VH	VH	L	M

1 Endpoint not evaluated with a score by the US EPA

2 No systemic toxicity or neurotoxicity based on single exposure reported by US EPA

3 No data located by US EPA

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

TABLE 8
SCORING OF TRIPHENYL PHOSPHATE USING THE PROPOSED MODIFIED ASSESSMENT/CLASSIFICATION METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	**L**	**L**	**L**	**H**	**L**	DG	**H**	DG	**L**	**L**	DG	**L**	**L**	**VH**	**VH**	**L**	**L**	1

Comments to hazard profile scores

As appears by comparison of the two tables, the two screening results for triphenyl phosphate are identical with the exception of the results for endocrine activity, bioaccumulation potential and skin irritation.

Several primary studies and a few secondary sources listed in the US EPA report (2014a) demonstrate effects on endocrine activity *in vitro* as well as *in vivo*. We have therefore assigned the score "High" to this endpoint (US EPA only presents data on endocrine activity, when available, but has not included scoring of this effect parameter)

Bioaccumulation was scored as "M" ("Moderate") by US EPA (2014a). However, based on the data presented this score is considered to be incorrect as none of the presented BCF's exceed a value of 500, which is the upper limit for a score as "Low". COWI therefore scores bioaccumulation potential as "L" based on the same data.

This result is in agreement with the evaluation and suggested small modifications of the GreenScreen® methodology to adapt it to a European context, which, with the exception of "Bioaccumulation", has led to only minor modifications of the original criteria limits and a moderate revision of the priority information sources to be used in the screening (as described in section 2.2).

For the particular example triphenyl phosphate, the mentioned modification of the "Bioaccumulation" criteria would not have had any impact on the hazard scoring anyway while use of the modified priority data sources (instead as the original data set, which was used here) theoretically could have affected the result slightly.

Overall hazard scoring
The US EPA substance profiles do not include an overall hazard score assessment as the GreenScreen® method does. Such a column is included in the modified substance summary table above to provide the full overview of the outcome of the substance assessment in one table. In the case of triphenyl phosphate, an overall hazard score = 1 is assigned because the substance meets criterion e) High T (Group I Human) by scoring "High" for endocrine activity.

3.3.2 Phenol, isobutylenated, phosphate (3:1), CAS No 68937-40-6

Isobutylenated phenol phosphate was used to test a new substance, i.e. a substance not previously assessed by the US EPA, using the modified GreenScreen® procedure.

The overall result of the data evaluation, i.e. the summary hazard table, is shown below while the full data set from the data collection including justification of the scoring based on the retrieved data is enclosed as Appendix 5 to this report.

TABLE 9
SCORING OF ISOBUTYLENATED PHENOL PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
DG	L	L	L	DG	H	DG	M	M	M	L	DG	M	M	VH	VH	L	M	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
Scoring of human health parameters are identical using the original GreenScreen® hazard criteria and the modified procedure for the endpoints where data have been identified. Information was not identified for carcinogenic properties, endocrine disruption, target organ toxicity from a single exposure, and respiratory sensitisation.

For the environmental parameters, only the scoring of Bioaccumulation potential would have been different if the original GreenScreen® hazard criteria had been applied as the BCFs in fish are in the interval from 1,000-2,000. The original GreenScreen® method has an upper limit of BCF = 1,000 for the "Moderate" criterion, and thus would have scored "High" for this substance, while the suggested modified method scores bioaccumulation potential as "Moderate" up to BCF = 2,000 (according to the lower limit for the B-criterion under REACH (PBT assessment)).

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not meet any of the criteria at Level 1 but meets criterion f) at Level 2 by scoring "very high" for ecotoxicity.

3.4 Applicability of the modified GreenScreen® methodology

The GreenScreen® methodology for screening hazard assessment of chemical substances was reviewed critically with the aim to assess whether the methodology could be of interest and would be possible to apply for such assessments in a European context, possibly with some modifications to be suggested.

The review revealed that despite having been developed in an American context, the GreenScreen® methodology is to a high degree aligned with both national and international regulations including the GHS and REACH, as well as national and international hazard lists and authoritative lists. Therefore, the suggested modifications of the methodology to adapt it to a European context are relatively minor and relate mainly to the data sources to be used for documentation and the relative priority of these, and a few changes of hazard classification intervals.

The hazard profiling methodology is considered to be applicable to human health and environmental hazard profiling of chemical substances in a European context. This is the case, not only for substances belonging to the group of flame retardants addressed in this project, but also for hazard profiling of chemicals of possible concern in general, extending beyond consumer product projects with possible additional, minor modifications. If the aim of the assessment is to identify possible alternatives to a given chemical, it is recommended to start with a rough overall hazard scoring assessment based on the List Translator before starting to prepare a full hazard profile for a substance.

However, the authors of this report find that hazard profiling using this screening tool requires persons with solid professional capability and experience within toxicology/human health assessment and environmental assessment in order to obtain reliable, balanced substance profiles, not least when assessing substances with incomplete data sets or with conflicting data for the same effect parameter. Additionally, in some cases it may be necessary to generate estimate data by use of QSAR modelling tools, which can require special expertise.

As regards the benchmarking part of the methodology, the criteria at Benchmark 1 level (BM1, i.e. the "worst" substances) are found to be aligned to a large extent with REACH SVHC criteria, with the exception that also a "very high" score for toxicity in Group II Human or "high" score in Group II* Human in combination with vP or vB lead to BM =1 in the GreenScreen® methodology. This is considered a relevant addition to the REACH SVHC criteria when the focus is on consumer products. Whether this exception is covered by the REACH SVHC criteria regarding Equivalent Level of Concern has not been assessed.

Benchmark scoring is possible even if data are not available for all hazard endpoints. E.g. data on sensitization are not necessary in order to score at the second highest benchmark level (BM3), however scoring at the highest level (BM4, i.e. the "best" substances) is only permissible for substances where data for all endpoints exist.

The exercise of overall hazard scoring of the 28 substances (individual results presented in the following chapter) revealed that the majority of the substances ended up in the same category and, thus, the differentiation between the substances appear to be too low to be really operational in a substitution situation. The exercise further showed that this, at least to some extent, was caused by a "gap" between two criteria levels (BM1 and BM2, see Table 4 for definitions) resulting in some substances obtaining an overall hazard score that does not fully reflect the hazard potential. Hence, for future occasions an additional benchmark level ("BM1½") could in principle be relevant to introduce. However, neither BM1½ nor BM2 substances are in reality very relevant to consider as possible long-term alternatives due to the nature and magnitude of the hazards covered by these two categories.

Finally, it should be noted that in a substitution decision-making situation, the hazard profile of a substance cannot stand alone but must be complemented by exposure considerations for relevant use scenarios. This could result in considering that for a specific scenario more weight should be put on some endpoints than others. E.g. in most consumer product contexts "acute toxicity" will not be a relevant endpoint because such concentrations are not likely to occur in reality and, consequently, this endpoint should evaluated on a case-by-case basis and possibly be neglected or at least be given lower weight than chronic endpoints. In other situations environmental endpoints could be assessed less relevant than human health endpoints for a particular scenario.

4. Hazard profiles and application data for flame retardants

This chapter presents hazard profiles for 28 marketed phosphorous flame retardants and five of the main halogenated flame retardants based on the modified GreenScreen® method.

Application profiles of marketed phosphorous flame retardants
The application profiles include for each of the marketed phosphorous flame retardants information on:

- CAS No, chemical name, structural formula, general formula, phosphorous content, abbreviations, product names, manufacturers, registered tonnage
- Applicability for each of the substrates as indicated in Pinfa's Product Selector (applicable, could be applied, etc.)
- Substrates (type of plastics, paint, textiles, etc.) as indicated by the manufacturers
- End applications (automotive, building, etc.) as indicated by manufacturers
- Interaction with substrate (additive, reactive)
- Environmental/health profiles: References to the US EPA DfE reports and screenings carried out in this project.
- Availability (recently introduced, widely applied, main flame retardant for the applications, etc.) to the extent data are available from manufacturers or the literature.
- Flame retardancy: Various information on the ability of the flame retardants in meeting different fire safety standards for relevant substrates as indicated in the literature, technical data sheets, etc. The description built on the information readily available for each flame retardant and is not systematically using the same methodology.
- Halogen-containing flame retardants for the same application to the extent it is described in the literature or in the manufacturer's product selectors. The list of halogen-containing flame retardants is not considered comprehensive, but includes examples identified.

The data are collected from technical data sheets and safety data sheets (SDSs) from the manufacturer's websites, as well as from literature with evaluations of flame retardants (references indicated in the tables).

Hazard profiles
Based on the methodology described in Chapter 3, modified GreenScreen profiles have been developed for 23 phosphorous flame retardants evaluated by the US EPA.

In addition to these, five "new" flame retardants (i.e. not previously evaluated by the US EPA) were selected for hazard screening as part of this study. The five flame retardants were selected from the long list based on the following criteria:

- The substance is already to some extent used as an alternative to halogenated flame retardants or marketed specifically as such.
- The substance meets the applicable fire safety requirement for major applications of the halogenated flame retardants
- The substance is registered under REACH, or significant environmental and health data are available otherwise

- The substance is not classified as a CMR substance in accordance with the CLP Regulation (Regulation (EC) No 1272/2008)

When available, information on environmental transformation products of the substances (or group of substances) has, in accordance with the GreenScreen® procedure, been taken into account when scoring the different endpoints to produce a hazard profile for one of the new substances. E.g. for melamine phosphate (CAS No. 41583-09-9), much of the data are based on tests with pure melamine and not the phosphate derivative. In the datasheet for melamine phosphate (Appendix 7), it is stated for each of the data provided when they are based on pure melamine rather than on the phosphate derivative.

The existing hazard profiles for the substances evaluated by US EPA mention transformation products where such have been identified, and where the hazards scores of these deviate from those of the parent compound. However, no full data sheets on transformation products are provided by US EPA and, hence, it has not been possible within the framework of the present study to fully evaluate a parameter such as endocrine disruption (ED), which is not included in the US EPA profile. However, where data indicate identification of transformation products, such as resorcinol in relation to RDP, these have been included in the screening.

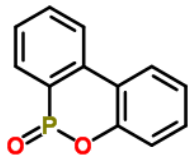
If also considering theoretical transformation products, such as bisphenol A in relation to BAPP, bisphenol A would score "high" for ED based on the adapted criteria. This would result in an overall hazard score 1 for flame retardants eventually resulting in transformation products such as bisphenol A, which is lower than the current scores.

In additions to the screening profiles, an overall hazard score has been calculated and is presented for each of the screened substances.

4.1 Organophosphorous compounds

4.1.1 DOPO, CAS No. 35948-25-5

Technical description

CAS No	35948-25-5
EC No	252-813-7
Chemical name	9,10-Dihydro-9-oxa-10-phosphaphenanthren-10-oxide
Structural formula	 Registration
General formula	C12H9O2P
Phosphorous content	14.0 – 14.6 (Metadynea)
Abbreviation, synonyms	DOPO; 6H-dibenz[c,e][1,2]oxaphosphorin-6-oxide
FR products and manufacturers	KCCS DO11, Metadynea EVERFOS DOPO, Everkem Mileflame DOPO, MPI Chemie
Registered tonnage, t/year	1,000 - 10,000

Pinfa Product Selector	Group Thermosets	Substrate Epoxy resins	Applicability Applicable
Other information on substrate	Evrfoss: ABS, flexible PUR, unsaturated polyester, epoxy resin, phenolic resins Metadynea: "DO11 is especially suited for polyesters and epoxy-systems, where DO11 is used as intermediate. It is s most effective as flame retardant where a gas / vapour phase radical inhibitor is required"		
End applications	Electrical and electronic equipment (EEE), transportation, wire and cable building and construction.		
Reactive/additive	Reactive		
Health env. profiles	Alternatives to TBBPA in printed CB (US EPA 2014c)		
Availability	Available from several manufacturers		
Flame retardancy	DOPO has been used as a flame retardant for certain types of printed wiring boards (Morose, 2006). UL 94-V0 rating of printed wiring boards was reached with 1.6 - 2.2% P-loading depending on substrates (Rakotamala et al., 2010). DOPO is the first efficient halogen free flame retardant for novolac-based epoxy systems (Rakotamala et al., 2010).		
Halogen-containing flame retardants for the same application (examples)	TBBPA used reactively		

Hazard profile

The screening of DOPO by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives to the halogenated flame retardant in printed circuit boards (US EPA, 2014c).

TABLE 10
SCORING DOPO USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	**L**	L	M	DG	L	DG	L	DG	M	M	DG	**L**	**M**	L	M	H	VL	2

Comments to hazard profile scores

The US EPA scores for Group I human toxicity are “moderate” for carcinogenicity and developmental toxicity due to an uncertain concern for adverse effects based on analogy with similar structures. Reproductive toxicity is scored as “low” based on analogy and professional judgement, and mutagenicity/genotoxicity is scored as “low” based on negative results from different *in vitro* studies. For Group II human toxicity systemic toxicity in one repeat dose study is available resulting in a “low” score based on the NOAEL established at the highest dose tested. The potential for neurotoxicity is scored as “moderate” based on structural alerts and professional judgement. No data is available for endocrine disruption and respiratory sensitization. Skin sensitization is scored a “moderate” due to limited data except for results from a local lymph node assay starting at 5%. Skin irritation was scored as “low” based on no skin reactions in an OECD test and eye irritation was scored as “moderate” based on moderate signs of eye irritation clearing in 7 days.

The US EPA score for persistence in the environment is "high" based on estimated data leading to an assessment of the half-life for ultimate degradation in soil of 75 days. However, the origin of this value is unclear as it is not included in the data table but only appears in the text justifying the

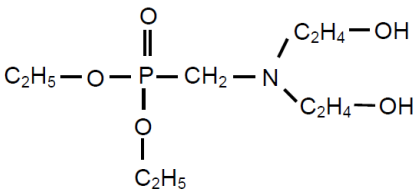
score. As, on the other hand, it is not obvious that the score for persistence should only be "moderate", the "high" score is maintained here.

No changes have been made to the US EPA hazard scores except for skin irritation and bioaccumulation, where the US EPA score was changed from “very low” to “low” and "low" to "very low", respectively. This is not because of a different assessment of the data, but merely because of a different categorization of the criteria in the original and the modified methodology.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind the overall hazard score = 1 but meets criterion e) for the overall hazard score = 2 by scoring "moderate" for both carcinogenicity and developmental effects in Group I Human.

4.1.2 N,N-bis-(2-hydroxylethyl) aminomethane phosphonic acid diethyl ester, CAS No. 2781-11-5

Technical description

CAS No	2781-11-5		
EC No	220-482-8		
Chemical name	N,N-bis-(2-hydroxylethyl) aminomethane phosphonic acid diethyl ester		
Structural formula	 Fyrol™ 6 datasheet		
General formula	C9H22NO5P		
Phosphorous content	12.1 % (Levagard 4090 N) 12.4 % (Fyrol™ 6)		
Abbreviation, synonyms	Diethyl bis(2-hydroxyethyl) aminomethylphosphonate		
FR products and manufacturers	Levagard 4090 N (Lanxess) Fyrol™ 6 (ICL-IP Europe)		
Registered tonnage, t/year	Pre-registered		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Foams	PUR rigid foam	Applicable
		PUR flexible foams	Applicable
	Thermosets	Phenolic resins	Applicable
Other information on substrate	Rigid PUR foams, PF, EP and UP resins		
End applications	"Levagard® 4090 N is especially suitable as flame retardant for rigid PUR foams. The product can support a closed-cell foam structure and can be combined with other Levagard or Disflamoll products. Further applications are possible in PF, EP and UP resins" (Lanxess)		
Reactive/additive	Reactive phosphonate ester which is incorporated into the foam structure by reacting as a polyol		
Health env. profiles	alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).		
Availability	Available from several manufacturers. The product is mainly used in rigid		

	PUR foams. Only used in flexible PUR foam in niche applications at the moment (Lassen et al., 2015)
Flame retardancy	Can be formulated to provide flame retardancy in spray, froth, pour-in-place and quasi pre-polymer applications, as well as the flame lamination of fabric with flexible foams (ICL-IP Europe).
Halogen-containing flame retardants for the same application (examples)	TCDP, TCPP

Hazard profile

The screening of N,N-bis-(2-hydroxylethyl) aminomethane phosphonic acid diethyl ester by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 11
SCORING N,N-BIS-(2-HYDROXYLETHYL) AMINOMETHANE PHOSPHONIC ACID DIETHYL ESTER USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	**M**	**L**	**L**	DG	**L**	DG	M	DG	M	M	DG	L	**L**	**M**	**L**	**H**	L	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

Data for three structurally similar analogs indicate evidence of carcinogenicity in laboratory animals and the uncertainty based on lack of studies on the substance compound leads to a “moderate” hazard designation by the US EPA. Conflicting results in tests with the commercial product (positive/negative) lead to a “moderate” score for mutagenicity/genotoxicity.

For most of the human health and ecotoxicity endpoints, experimental data for a commercial product (Fyrol 6) are available in the US EPA report (2015). The evaluation of potential for neurotoxicity, repeated dose effects and skin sensitization were based on either structural alerts (organophosphates, amines) and/or professional judgement.

The evaluation of irritation of eye and skin is based on experimental data from rabbit studies.

No data were available for endocrine activity and respiratory sensitization.

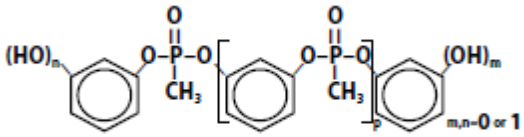
The bioaccumulation score is based on QSAR estimations.

Overall hazard scoring

An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1 but meets criterion c) for Benchmark 2 by scoring “high” in persistence and "moderate" for several endpoints in Group I, II and II* Human.

4.1.3 Poly(m-phenylene methylphosphonate), CAS No. 63747-58-0

Technical description

CAS No	63747-58-0
EC No	*613-366-7
Chemical name	Poly(m-phenylene methylphosphonate)
Structural formula	 ICL-IP Europe product catalogue
General formula	(C13H13O3P · C6H6O2)x
Phosphorous content	17.5 % (Fyrol PMP)
Abbreviation, synonyms	DEEP
FR products and manufacturers	Fyrol PMP (ICL-IP Europe)
Registered tonnage, t/year	Pre-registered
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Epoxy resins (ICL-IP Europe)
End applications	EEE
Reactive/additive	Reactive
Health env. profiles	Alternatives to the halogenated flame retardant in printed circuit boards (US EPA, 2014b)
Availability	Have been on the market for several years and applied for printed wiring boards.
Flame retardancy	FR-4 laminates with Fyrol PMP are marketed (Morose, 2006) When a novolac epoxy resin is cured with Fyrol PMP (20 wt %) in presence of ATH (35 wt %) a UL 94-V0 rating can be reached (Rakotamala et al.,2010).
Halogen-containing flame retardants for the same application (examples)	TBBPA (used reactively)

Hazard profile

The screening of Poly(m-phenylene methylphosphonate) by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives to the halogenated flame retardant in printed circuit boards (US EPA, 2014b).

TABLE 12
SCORING OF POLY(M-PHENYLENE METHYLPHOSPHONATE) USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	M	M	H	L	DG	M	DG	M	L	DG	L	L	H	H	VH	H	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
The US EPA scores for Group I human toxicity are "low" for carcinogenicity and genotoxicity based on analogy with similar structures and professional judgment. Reproductive toxicity as well as mutagenicity/genotoxicity are scored as "medium" based on data for a confidential analogue and professional judgement. The score for systemic toxicity is based on analogy to RDP (CASRN 125997-21-9), a confidential analogue and professional judgement.

There are no experimental data for endocrine activity in the report, however, resorcinol (CAS Nr 108-46-3), a metabolite of the analogue RDP and a starting material in Fyrol PMP synthesis, is listed as a Cat. 1 (Evidence for endocrine disruption in living organisms) substance on the priority list by the EU. COWI therefore assigns the score "high" to this endpoint.

With respect to neurotoxic effects, the "moderate" score is derived from extrapolation from a 28-day study for the analogue RDP (CASRN 125997-21-9). There is also potential for neurotoxicity based on the presence of the phenol and organophosphorus structural alerts.

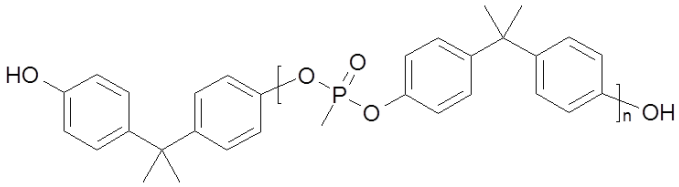
No data were available for respiratory sensitization.

The high MW components with a MW>1,000 have low water solubility and are expected to have no effects at saturation. However, QSAR estimations for the ECOSAR class of phenols of the n = 1 oligomers result in LC50 values low enough to cause "high" aquatic toxicity scores. Since the n = 1 oligomer constitutes only a fraction of the polymer mixture (more exact data on polymer composition are not available) and the estimations are based on a compound class and not a specific compound, we regard the score as protective. Correspondingly, only two oligomers (n = 3 and 4) cause the bioaccumulation score "high", while the other components of the polymer mixture have moderate or low potential to bioaccumulate.

Overall hazard scoring
An overall hazard score = 1 has been assigned because the substance scores "High" for the endpoints endocrine activity, acute and chronic aquatic toxicity, as well as for bioaccumulation. Furthermore, the substance scores "Very high" for persistence.

4.1.4 Phosphonate oligomers, CAS No. 68664-06-2

Technical description

CAS No	68664-06-2		
EC No	Not available		
Chemical name	Phosphonate oligomers		
Structural formula	 Representative structure (US EPA 2014a)		
General formula	C15H16O2(C16H17O3P)n		
Phosphorous content	8.5 % (NOFIA™ OL1001) 10 % (NOFIA™ OL3001)		
Abbreviation, synonyms			
FR products and manufacturers	NOFIA™ OL1001, NOFIA™ OL3001 (FRX Polymers)		
Registered tonnage, t/year	Not reg/pre-reg		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastics	Thermoplastic elastomers	Applicable
	Foams	Rubbers/elastomers	Applicable
	Thermosets	Unsaturated polyesters	Applicable
		Epoxy resin	Applicable
	Wires and cables	TPU	Applicable
Other information on substrate	Unsaturated polyesters, epoxy, PUR and polyurea		
End applications	Decorative laminates, wall panels, copper clad laminates for printed circuit boards, protective sheets and coatings, adhesives (FRX Polymers)		
Reactive/additive	Reactive		
Health env. profiles	Alternatives for the flame retardant decaBDE (US EPA, 2014a)		
Availability	-		
Flame retardancy	-		
Halogen-containing flame retardants for the same application (examples)	DecaBDE, TBBPA		

Hazard profile

The screening of Phosphonate oligomers by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 13
SCORING PHOSPHONATE OLIGOMERS USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	L	L	DG	L	L	L	M	M	L	DG	M	M	L	H	VH	H	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
No data on carcinogenicity have been located in the US EPA report leading to the conclusion that carcinogenic effects cannot be ruled out. The US EPA estimates the potential for mutagenicity/ genotoxicity of the phosphonate oligomer as low based on analogy to BAPP (CAS no. 181028-79-5)

Based on professional judgement, limited bioavailability and the absence of structural alerts, the potential for reproductive and developmental effects were estimated as low. The score (moderate) for neurotoxicity and irritation of skin and eye is based on the presence of the phenol structural alert.

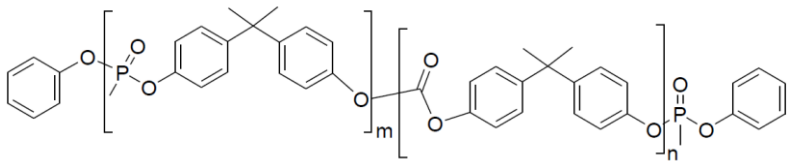
With respect to endocrine activity and respiratory sensitization, no studies were available.

The scores for aquatic toxicity and persistence are based on professional judgement and QSAR estimations. The "high" score for chronic aquatic toxicity results from estimation on the n=1 and n=2 oligomers. Both measured and estimated data are available for the evaluation of bioaccumulation.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1. However, since the overall hazard 2 criterion b) only requires high P and high B, while the substance scores "very high" in P and also "high" in T, the overall hazard score 2 does not fully reflect the hazard potential of the substance.

4.1.5 Poly[phosphonate-co-carbonate], CAS No. 77226-90-5

Technical description

CAS No	77226-90-5		
EC No	Not available		
Chemical name	Poly[phosphonate-co-carbonate]		
Structural formula	 Representative structure (US EPA 2014a)		
General formula	C15H16O2(C16H14O3)n(C16H17O3P)m		
Phosphorous content	No data		
Abbreviation, synonyms	Carbonic acid, diphenyl ester, polymer with diphenyl P-methylphosphonate and 4,4'- (1-methylethylidene)bis[phenol]		
FR products and manufacturers	NOFIA™ CO6000 (FRX Polymers)		
Registered tonnage, t/year	Not reg/pre-reg		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastics	HIPS/PPO	Applicable
		PC/ABS	Applicable
		Polycarbonate (PC)	Applicable
Other information on substrate	None		
End applications	"Thin, transparent, high flow molding EE&CE applications and extruded films and sheet for B&C applications" (FRX Polymers)		
Reactive/additive	Additive		
Health env. profiles	Alternatives for the flame retardant decaBDE (US EPA, 2014a)		
Availability	-		
Flame retardancy	UL 94 V0 grades of polycarbonate and polycarbonate blends		
Halogen-containing flame retardants for the same application (examples)	TBBPA, proprietary polymeric FR		

Hazard profile

The screening of poly[phosphonate-co-carbonate] by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 14
SCORING POLY[PHOSPHONATE-CO-CARBONATE] USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	L	L	L	L	L	L	L	L	L	DG	L	L	L	L	VH	L	3

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

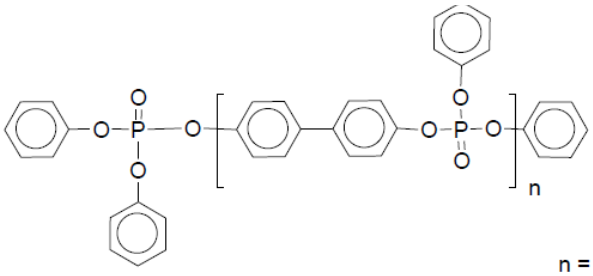
Comments to hazard profile scores
Only very limited measured data are available in the US EPA report. However, because of the large size of the polymer (MW >1,000), it is expected to have limited bioavailability and metabolism in the human body. Therefore, the potential for human health effects is low based on professional judgement.

Correspondingly, the large MW, limited bioavailability and low water solubility suggest that there will be no effects on the aquatic environment at saturation. The polymer is not expected to be removed by biodegradation or other degradative processes under environmental conditions because of limited bioavailability, limited water solubility and limited partitioning to air.

Overall hazard scoring
An overall hazard score = 3 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1 or 2. However, since the overall hazard 3 criterion a) only requires moderate P or B, while the substance scores “very high” in P, the overall hazard score 3 does not fully reflect the hazard potential of the substance.

4.1.6 Phosphoric acid, mixed esters with [1,1'-bisphenyl-4,4'-diol] and phenol, CAS No. 1003300-73-9

Technical description

CAS No	1003300-73-9		
EC No	Not available		
Chemical name	Phosphoric acid, mixed esters with [1,1'-bisphenyl-4,4'-diol] and phenol		
Structural formula	 US EPA 2014a		
General formula	$C_{36}H_{28}O_8P_2$ (n = 1)		
Phosphorous content	No data		
Abbreviation, synonyms	BPBP		
FR products and manufacturers	ADK STAB FP-800 (Adeka Palmerole)		
Registered tonnage, t/year	Not reg/pre-reg		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastics	HIPS/PPO	Applicable
		PC/ABS	Applicable
		Polycarbonate (PC)	Applicable
	Textiles/paints/adhesives	Other textile fibers	Applicable
	Wire and cables	TPU	Applicable
Other information on substrate	Polycarbonates and polyesters, polymer blends such as PC/ABS and PC/HIPS.		
End applications	-		
Reactive/additive	Additive		
Health env. profiles	Evaluated in this study (see below)		
Availability	-		
Flame retardancy	-		
Halogen-containing flame retardants for the same application (examples)	DecaBDE, TBBPA, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others		

Hazard profile

The screening of phosphoric acid, mixed esters with [1,1'-bisphenyl-4,4'-diol] and phenol (BPBP) by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 15
SCORING PHOSPHORIC ACID, MIXED ESTERS WITH [1,1'-BISPHENYL-4,4'-DIOL] AND PHENOL USING THE PROPOSED MODIFIED METHODOLOGY.

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	**L**	L	L	DG	**L**	DG	**L**	DG	**L**	**L**	DG	VL	VL	H	H	**H**	L	

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
BPBP is a polymer mixture mainly consisting of the n = 1 oligomers (> 80% of the composition).

In the absence of experimental data, the carcinogenic potential of BPBP was precautiously scored as "moderate", even though neither structural alerts nor read-across from an analogue indicate carcinogenicity. *In vitro* studies showed that BPBP is not mutagenic.

No data were available for the endpoints endocrine disruption and respiratory sensitization.

A single 28-day oral neurotoxicity screening study lead to the conclusion of low neurotoxic potential in the US EPA report. However, the authors also state that there is uncertainty due to lack of data on cholinesterase inhibition, which is an effect associated with phosphate esters.

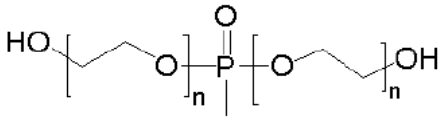
With respect to aquatic toxicity, several experimental studies with BPBP report EC50/LC50 values above the water solubility limit without providing further study details, thus indicating no effects at saturation. QSAR estimations for the compound class of neutral organics yield very low LC50 values (< 0.01), but professional judgement indicates that this compound does not lie within the domain of the ECOSAR model. A single experimental study in algae with a structurally similar, but confidential analogue yields very low effect concentrations (EC50 value of <1.0 mg/L and NOEC < 0.1 mg/L), causing the assignment of the "high" score for the aquatic toxicity endpoints. Based on a conservative approach, the assessment is adopted in our evaluation.

A single experimental study, QSAR estimations and professional judgement on biotic and abiotic degradation lead to the conclusion that the substance is not easily removed under environmental conditions. With respect to bioaccumulation, our score (low) deviates according to CLP criteria from the evaluation by the US EPA, who assigned the score "moderate" based on a QSAR-estimated BCF of 172.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1. The overall hazard 2 criterion c) requires only high P and moderate T (Ecotoxicity or Group I, II or II* Human), while the substance scores "high" in T (ecotox.). However, considering the conservative approach in evaluating ecotoxicity, the Benchmark score 2 presumably reflects the hazard potential of the substance sufficiently.

4.1.7 Oligomeric phosphonate polyol, CAS No. 363626-50-0

Technical description

CAS No	363626-50-0
EC No	Not available
Chemical name	Oligomeric phosphonate polyol
Structural formula	 US EPA 2015
General formula	CH5O3P·(C2H4O)n·(C2H4O)n
Phosphorous content	10 - 13% (Exolit® OP 560)
Abbreviation, synonyms	
FR products and manufacturers	Exolit® OP 560, Exolit® OP 550 (Clariant)
Registered tonnage, t/year	Neither registered nor pre-registered
Pinfa Product Selector	Group: Substrate: Applicability:
Other information on substrate	Flexible polyurethane foams
End applications	Automotive industry
Reactive/additive	Reactive
Health env. profiles	Alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).
Availability	The product has been marketed for more than 10 years. The FR seems in particular to be used together with PUR foam with a "green" polyurethane foam technology partly based on biomass-derived natural oil polyols and according to the manufacturer, Exolit, OP types FRs are especially suited for these polyols
Flame retardancy	Reactive flame retardant (phosphor-based polyol) i.e. it is incorporated into a polymer backbone (e.g. polyurethane) by chemically bonding with raw materials during the polymerization process. The concentration of Exolit OP 560 is about 20% of the level of non-reactive FRs, which would normally be required to pass the Californian standard Cal 117 for furniture (Lassen et al., 2015) No data regarding meeting the UK Crib 5 test for furniture has been identified. Some informal information has indicated that with this FR it would be more challenging to develop foams that can pass the UK Crib 5 test as compared with the Cal 117 (Lassen et al. 2015).
Halogen-containing flame retardants for the same application (examples)	TCCP; TDCP in flexible PUR foams

Hazard profile

The screening of oligomeric phosphonate polyol by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 16
SCORING OF PHOSPHORUS POLYOL USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	M	L	M	DG	**L**	L	L	M	M	L	DG	L	L	**L**	M	**M**	L	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

There is uncertainty due to lack of experimental data on carcinogenicity and genotoxicity for this substance; those effects can therefore not be ruled out. The scoring of reproductive and developmental potential, neurotoxicity, repeated dose effects and skin sensitization is based on professional judgement and structural alerts (organophosphates).

No data were available for the endpoints endocrine disruption and respiratory sensitization.

Only few experimental data were available for aquatic toxicity; the evaluation is therefore supported by QSAR and professional judgement based on read-across.

The bioaccumulation score is based on solely QSAR estimations, while a few experimental studies also support the conclusion on persistence.

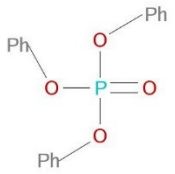
Overall hazard scoring

An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1 but meets criterion e) for Benchmark 2 by scoring “moderate” for several endpoints in Group I Human.

4.2 Organophosphates (phosphate esters) – Aryl phosphates

4.2.1 Triphenyl phosphate, CAS No. 115-86-6

Technical description

CAS No	115-86-6		
EC No	204-112-2		
Chemical name	Triphenyl phosphate		
Structural formula	 Registration		
General formula	C18H15O4P		
Phosphorous content	9.5% (EVERFOS TP (TPP); Disflamoll TP; Disflamoll TP Liquid)		
Abbreviation, synonyms	TPP, TPHP		
FR products and manufacturers	EVERFOS TP (TPP) (Everkem) Disflamoll TP, Disflamoll TP liquid (Lanxess)		
Registered tonnage, t/year	1,000 – 10,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastics	HIPS/PPO	Applicable
		PC/ABS	Applicable
	Thermosets	Phenolic resins	Applicable
		Epoxy resins	Applicable
Other information on substrate	PP, PE, PVC, HIPS, PC/ABS (alloys), PPO/HIPS (alloys), rigid and flexible polyurethane, TPU, Epoxy resin, phenolics resin, PC, textile (back coating), adhesive, rubbers, cellulose acetate, cellulose acetate butyrate and vinyl copolymer, PPE/HIPS		
End applications	Moulding applications, coatings, EEE		
Reactive/additive	Additive		
Health env. profiles	Alternatives to decaBDE (US EPA, 2015); flame retardants to flexible PUR foams (US EPA, 2014b)		
Availability	Have been available for many years from several manufacturers		
Flame retardancy	When using phosphorous flame retardants to substitute for HIPS with decaBDE it has been necessary to replace the HIPS with the copolymers PC/ABS and HIPS/PPO in order to meet the requirements in casings of EEE (Lassen et al., 2007; Illinois EPA, 2007). Loading of 8-12% in PC/ABS in order to prepare V-0 grade PC/ABS for EEE (Lassen et al., 2006).		
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others		

Hazard profile

The screening of triphenyl phosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives to the flame retardant decaBDE (US EPA, 2014a).

TABLE 17
SCORING OF TRIPHENYL PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	**L**	**L**	**L**	**H**	**L**	DG	**H**	DG	**L**	**L**	DG	**L**	**L**	**VH**	**VH**	**L**	**L**	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores.

Experimental data are available for all human toxicity endpoints apart from respiratory sensitization in the US EPA report, often referred from reliable secondary sources.

The US EPA does not assign a score on the endpoint of endocrine activity. However, several primary studies and a few secondary sources listed in the report demonstrate effects on endocrine activity *in vitro* as well as *in vivo*. We therefore assign the score "High" to this endpoint.

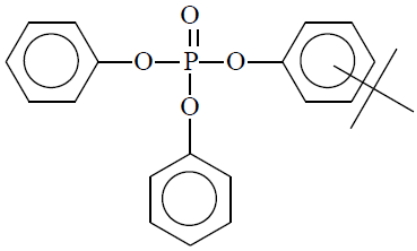
Bioaccumulation was scored as "M" ("Moderate") by US EPA (2014a). However, based on the data presented this is considered be incorrect as none of the presented BCF's exceed a value of 500, which is the upper limit for a score as "Low". COWI therefore scores bioaccumulation potential as "L" based on the same data.

Overall hazard scoring

An overall hazard score = 1 has been assigned because the substance meets criterion e) of Benchmark 1: High T (Group Human I).

4.2.2 Phenol, isobutylenated, phosphate (3:1), CAS No. 68937-40-6

Technical description

CAS No	68937-40-6
EC No	273-065-8 / 700-990-0
Chemical name	Phenol, isobutylenated, phosphate (3:1)
Structural formula	 Reofos® LF-50 data sheet
General formula	
Phosphorous content	8.4% (Reofos® LF-50)
Abbreviation, synonyms	Reaction mass of 4-tert-butylphenyl diphenyl phosphate and bis(4-tertbutylphenyl) phenyl phosphate and triphenyl phosphate
FR products and manufacturers	Reofos® LF-50 (Green Lake Solutions) Disflamoll TP LXS 51092 (Lanxess)
Registered tonnage, t/year	1,000 – 10,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	PVC, flexible polyurethanes, cellulosic resins, and synthetic rubber. Flame retardant processing aid for engineering resins, such as modified PPO, polycarbonate and polycarbonate blends
End applications	-
Reactive/additive	Additive
Health env. profiles	Screened as part of this study (see below)
Availability	-
Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	TCPP

Hazard profile

The screening of this alternative by the modified GreenScreen® methodology was based on information compiled according to the information sources described in 3.2.1. The full data set from the data collection including justification of the scoring is enclosed as Appendix 5 to this report.

TABLE 18
SCORING OF PHENOL, ISOBUTYLENATED, PHOSPHATE (3:1) USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
DG	L	L	L	DG	L	DG	M	M	M	L	DG	M	M	VH	VH	L	M	2

Comments to hazard profile scores
According to REACH registration, Phenol, isobutylenated, phosphate is made up of four different constituents: p-t-butylphenyl diphenyl phosphate, bis(p-t-butylphenyl) phenyl phosphate, tris(p-tert-butylphenyl) phosphate and triphenyl phosphate. Furthermore, some tests were made with commercial products. Data on the components as well as on the commercial products are considered in the screening.

A notified classification is available for Phenol, isobutylenated, phosphate (3:1); Aquatic Chronic 1 (H410; 1 notifier) and Aquatic Chronic 3 (H412; 1 notifier).

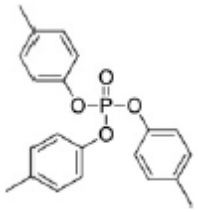
Information was not identified for carcinogenic properties, endocrine disruption, target organ toxicity from a single exposure, and respiratory sensitization. For all other human endpoints as well as aquatic toxicity, experimental data were available.

A single biodegradability study allowed for the evaluating of persistence while the scoring of bioaccumulation potential is based on both measured and estimated data.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not meet any of the criteria at Level 1 but meets criterion f) at Level 2 by scoring "very high" for ecotoxicity.

4.2.3 Tricresyl phosphate, CAS No. 1330-78-5

Technical description

CAS No	1330-78-5		
EC No	215-548-8		
Chemical name	Tricresyl phosphate		
Structural formula	 Bergman et al. 2012		
General formula	$C_{21}H_{21}O_4P$		
Phosphorous content	8.4% (Everfos TCP); Disflamoll TKP, Disflamoll TKP-P; Kronitex TCP)		
Abbreviation, synonyms	TMPP; Tris(methylphenyl) phosphate, TCP		
FR products and manufacturers	EVERFOS TCP (Everkem) Kronitex® TCP (Great Lake Solutions) Disflamoll TKP (Lanxess) Disflamoll TKP-P (Lanxess)		
Registered tonnage, t/year	1,000 – 10,000		
Pinfa Product Selector	Group: Wires and cables	Substrate: PVC flexible	Applicability: Applicable
Other information on substrate	PVC, PVC flexible, polyester, phenolics resin, nitrocellulose lacquers and coatings and processing aid for natural and synthetic rubbers (NBR and SBR)		
End applications	Wires and cables, building materials		
Reactive/additive	Additive		
Health env. profiles	Alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015)		
Availability	Available from manufacturers		
Flame retardancy	-		
Halogen-containing flame retardants for the same application (examples)	DBDPE, EBTEBPI, TCPP		

Hazard profile

The screening of tricresyl phosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 19
SCORING TRICRESYL PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
The alternative tricresyl phosphate may contain a mixture of methylated triphenyl phosphate isomers with an unspecified degree of methyl substitution. Therefore, 12 closely related compounds were included in the assessment by the US EPA.

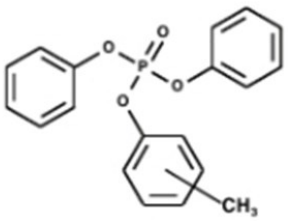
Experimental data for tricresyl phosphate are available for all human health endpoints apart from respiratory sensitization. Most conclusions on the respective endpoints are based on experiments with a commercial mixture of the substance.

The evaluation of aquatic toxicity, persistence and bioaccumulation was based on experimental data supported by QSAR estimations. Ten out of the 11 available factors for bioconcentration/-accumulation do not exceed > 2000, which is the lower margin for the "high" according to CLP criteria. However, considering the available measured log Kow values (5.11, 5.9, 4.51, and 3.7) and a conservative approach, the "high" score assigned by the US EPA is also applied in our evaluation.

Overall hazard scoring
An overall hazard score = 1 has been assigned because the substance fulfils the criterion e) behind Benchmark 1; High T (Group I Human).

4.2.4 Cresyl diphenyl phosphate, CAS No. 26444-49-5

Technical description

CAS No	26444-49-5		
EC No	247-693-8		
Chemical name	Cresyl diphenyl phosphate		
Structural formula	 Everkem product brochure		
General formula	C21H17O4P		
Phosphorous content	9.5% (EVERFOS CDP) 9.1% (Kronitex CDP; Disflamoll DPK)		
Abbreviation, synonyms	CDP		
FR products and manu-facturers	EVERFOS CDP (Everkem) Kronitex® CDP (Great Lakes Solution) Disflamoll DPK (Lanxess)		
Registered tonnage, t/year	Pre-registered		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastic	PC/ABS	Applicable
		HIPS/PPO	Applicable
		Thermoplastic elastomer	Applicable
	Foams	PVC/nitrile foam	Applicable
		PUR rigid foam	Could be applied
		Rubbers/elastomers	Applicable
	Textiles/paints/adhesives	Hot melts	Applicable
		Paints	Applicable
		Latex/adhesives	Applicable
	Thermosets	Phenolic resins	Applicable
	Wires and cables	PVC flexible	Applicable
		TPU	Applicable
		PE/EVA	Could be applied
Other information on substrate	PVC, flexible polyurethane, epoxy resin, phenolics resin, PC/ABS blends, TPU compounds, PUR- foams (rigid and flexible) and rubbers		
End applications	Electrical components, printed wiring board, building materials		
Reactive/additive	Additive		
Health env. profiles	Not included in US EPA screenings but a screening is prepared below based on an analogue substance		
Availability	Have been available for many years from several manufacturers		

Flame retardancy	Used in PC/ABS copolymers in casings for EEE (Lowell, 2005), but seems to be less used than other organophosphates (DBP, RDP, TPP) for this application.
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others may be used for some of the same applications. For the main application area in PVC application CDP is not used as an alternative to halogenated flame retardants.

Hazard profile

Cresyl diphenyl phosphate (CDP) is a structural analogue to and an impurity in TCP (CAS No. 1330-78-5, section 4.2.2), only differing in the methylation degree of the phenol moieties. Available substance data were included in the profile of TCP, and a separate screening of CDP is not available in the US EPA report (US EPA, 2015). We therefore suggest the same scoring for CDP as for TCP.

TABLE 20
SCORING OF CRESYL DIPHENYL PHOSPHATE BASED ON THE PROFILE FOR TCP.

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
See section 4.2.2.

Overall hazard scoring
Overall hazard score 1, see section 4.2.2.

4.2.5 Phosphoric acid, bis(methylphenyl) phenyl ester, CAS No. 26446-73-1

Technical description

CAS No	26446-73-1
EC No	247-708-8
Chemical name	Phosphoric acid, bis(methylphenyl) phenyl ester
Structural formula	-
General formula	-
Phosphorous content	-
Abbreviation, synonyms	Bis-(methylphenyl) phenyl phosphate
FR products and manufacturers	Not identified as manufactured. The substance is a structural analogue to and a impurity in TCP

Hazard profile

Phosphoric acid, bis(methylphenyl) phenyl ester is a structural analogue to and a impurity in TCP (CAS No. 1330-78-5, section 4.2.2), only differing in the methylation degree of the phenol moieties. Available substance data were included in the profile of TCP, and a separate screening of phosphoric acid, bis(methylphenyl) phenyl ester is not available in the US EPA report (US EPA, 2015). We therefore suggest the same scoring for phosphoric acid, bis(methylphenyl) phenyl ester as for TCP.

TABLE 21
SCORING OF PHOSPHORIC ACID, BIS(METHYLPHENYL) PHENYL ESTER BASED ON THE PROFILE FOR TCP.

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	H	M	DG	M	DG	H	DG	M	M	DG	L	L	VH	H	M	H	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

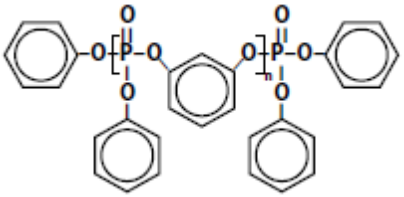
See section 4.2.2.

Overall hazard scoring

Overall hazard scorek 1, see section 4.2.2.

4.2.6 Resorcinol bis-diphenyl phosphate, CAS No. 57583-54-7

Technical description

CAS No	57583-54-7 (sometimes 125997-21-9 is used interchangeably)		
EC No	260-830-6		
Chemical name	Resorcinol bis-diphenyl phosphate		
Structural formula	 ICL-IP Europe product catalogue		
General formula	C30H24O8P2		
Phosphorous content	10.8% (EVERFOS RDP) 10.7% Fyrolflex RDP		
Abbreviation, synonyms	RDP, tetraphenyl m-phenylene bis(phosphate), tetraphenyl resorcinol bis-diphenyl phosphate, PBDPP		
FR products and manufacturers	EVERFOS RDP (Everkem) Fyrolflex RDP (ICL-IP Europe) AFLAMMIT® PLF 280 (THOR)		
Registered tonnage, t/year	1,000 – 10,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermosplastic	HIPS/PPO	Applicable
		PC/ABS	Applicable
		Polycarbonate (PC)	Applicable
		Polyamide (PA)	Applicable
		PBT	Applicable
		PET	Applicable
Other information on substrate	EPDM, HIPS, PC/ABS (alloys), PPE/HIPS (alloys), TPU, epoxy resin, PC, modified PPO,		
End applications	Automotive, EEE		
Reactive/additive	Additive		
Health env. profiles	Alternatives for the flame retardant decaBDE (US EPA, 2014a)		
Availability	Available from many manufacturers. RDP are widely used as flame retardant in casing of EEE made of the co-polymers PC/ABS and HIPS/PPO (Lassen et al., 2006)		
Flame retardancy	When using phosphorous flame retardants to substitute for HIPS with decaBDE it has been necessary to replace the HIPS with the copolymers PC/ABS and HIPS/PPO in order to meet the requirements in casings for EEE (Lassen et al., 2007; Illinois EPA, 2007). Loading 10-14% in order to prepare V-0 grade PC/ABS for EEE (Lassen et al., 2006)		
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others		

Hazard profile

The screening of resorcinol bis-diphenyl phosphate (RDP) by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 22
SCORING OF RESORCINOL BIS-DIPHENYL PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	L	M	H	L	DG	M	DG	M	L	DG	L	L	VH	VH	M	H	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

The score on acute mammalian toxicity is based on experimental data with RDP. Data on carcinogenicity were not located by the US EPA, but the carcinogenic potential is estimated to be moderate based on professional judgement. In contrast, several experimental studies were available for mutagenicity and genotoxicity, resulting in a low score for this endpoint.

Experimental data for resorcinol bis-diphenylphosphate indicate no adverse effects on reproductive performance or fertility parameters at the doses tested. However, the US EPA states that there may be potential for reproductive toxicity based on analogy to confidential analogue.

Resorcinol (CAS No 108-46-3), a metabolite of RDP, is listed as a Cat. 1 (Evidence for endocrine disruption in living organisms) substance on the priority list by the EU. We have therefore assigned the score "high" to this endpoint. With respect to neurotoxic effects, the "moderate" score is derived from extrapolation from a 28-day study. There is also potential for neurotoxicity based on the presence of organophosphates structural alerts. RDP produced mild irritation in rabbit eyes; however, effects were reversible within 24 hours.

An experimental study with daphnids suggests that the EC50 does not exceed water solubility, leading to the designation of "very high" scores for aquatic toxicity.

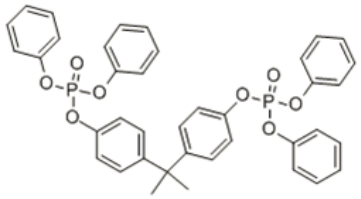
With respect to bioaccumulation, the US EPA assigns the score "high" based on a QSAR-estimated BCF of 1,300. This value would usually be regarded as "moderately" bioaccumulative according to CLP criteria. However, the Log Kow has been measured to 4.93 and 4.9 by two independent studies, thus triggering a "High" score for bioaccumulation. Since the US EPA report does not provide further details on whether the BCF QSAR estimate is based on measured or estimated log Kow values, we rely in our evaluation of bioaccumulation on the measured log Kow value, resulting in a "high" score.

Overall hazard scoring

An overall hazard score = 1 has been assigned because the substance fulfils criterion e) "high" T (Group I Human).

4.2.7 Bisphenol A bis(diphenyl phosphate), CAS No. 5945-33-5

Technical description

CAS No	5945-33-5 (sometimes 181028-79-5 is used interchangeable).		
EC No	425-220-8		
Chemical name	Bisphenol A bis(diphenyl phosphate)		
Structural formula	 Registration		
General formula	C39H34O8P2 (n = 1; CAS No. 5945-33-5)		
Phosphorous content	8.9% (Everfos BP (BDP); Fyrolflex BDP; ADK STAB FP-600)		
Abbreviation, synonyms	BPA-BDPP, BDP, BAPP; (1-methylethylidene)di-4,1-phenylenetetraphenyl diphosphate		
FR products and manufacturers	ADK STAB FP-600 (Adeka Palmarole) EVERFOS BP (BDP) (Everkem) Fyrolflex BDP (ICL-IP Europe)		
Registered tonnage, t/year	1,000 – 10,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastic	HIPS/PPO	Applicable
		PC/ABS	Applicable
		Polycarbonate (PC)	Applicable
	Textiles/paints/adhesives	Other textile fibres	Applicable
	Wires and cables	TPU	Applicable
Other information on substrate	EPDM, HIPS, PC/ABS (alloys), PPE/HIPS (alloys), TPU, epoxy resin, PC, HIPS/PPO		
End applications	EEE		
Reactive/additive	Additive		
Health env. profiles	Alternatives to decaBDE (US EPA, 2014a)		
Availability	Have been available from several manufacturers for many years. A major flame retardant for casings for EEE		
Flame retardancy	When using phosphorous flame retardants to substitute for HIPS with decaBDE it has been necessary to replace the HIPS with the copolymers PC/ABS and HIPS/PPO in order to meet the requirements in casings or EEE (Lassen et al., 2007; Illinois EPA, 2007). Loading 10-14% in order to obtain V-0 grade PC/ABS for EEE (Lassen et al., 2006)		
Halogen-containing flame retardants for the same application (examples)	Polybrominated styrenes/ brominated polystyrenes (main FR in PA), decaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others		

Hazard profile

The screening of bisphenol A bis(diphenyl phosphate) (BAPP) by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 23
SCORING OF BISPHENOL A BIS(DIPHENYL PHOSPHATE) USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	DG	L	DG	L	DG	L	DG	L	L	DG	L	L	L	L	H	M	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

The US EPA suggests that BAPP may have a low potential for carcinogenicity based on expert judgement and the absence of no structural alerts in the molecule. However, due to uncertainty caused by lack of data, the US EPA assigns a “moderate” score.

A single 28-day oral neurotoxicity screening study lead to the conclusion of low neurotoxic potential in the US EPA report. However, the authors also state that there is uncertainty due to lack of data on cholinesterase inhibition, which is an effect associated with phosphate esters.

With respect to reproductive effects, the US EPA report provides no data at all. The designation of “low” potential for reproductive effects is solely based on expert judgement without further justification. We have therefore marked this endpoint as data gap. Data are also lacking for the endpoints endocrine activity and respiratory sensitization. The potential for developmental effects is estimated to be low based on a structurally similar confidential analogue.

Experimental data indicate no effects on the aquatic environment at saturation. BAPP is neither readily biodegradable nor expected to be removed by abiotic degradation. With respect to bioaccumulation, our score ("moderate") deviates according to CLP criteria from the evaluation by the US EPA, who assigned the score “high” based on a QSAR-estimated BAF of 1,100.

Bisphenol A was not identified as a transformation product of BAPP by US EPA as such, but was mentioned as a possible transformation product, which would score differently than the parent compound for reproductive effects, skin sensitization and dermal irritation ("moderate" versus "low" for BAPP). However, the hazards of the theoretical degradation products including bisphenol A were not considered in the hazard profile for BAPP in the US EPA report and therefore endocrine disruption related to this substance has not been considered here.

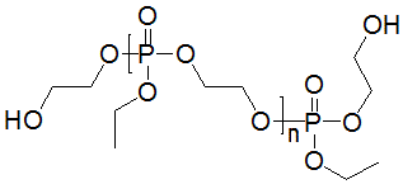
Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1, but meets criterion c) for Benchmark 2 by scoring "high" for persistence and “moderate” for carcinogenicity.

It is noted that inclusion of bisphenol A in the benchmarking would not have changed the assigned overall hazard score (2) (when not considering endocrine disruption properties for which data were not provided by US EPA).

4.3 Organophosphates (phosphate esters) – Alkyl phosphates

4.3.1 Oligomeric ethyl ethylene phosphate, CAS No. 184538-58-7

Technical description

CAS No	184538-58-7
EC No	*606-033-2
Chemical name	Oligomeric ethyl ethylene phosphate
Structural formula	 Representative structure (US EPA 2015)
General formula	(C6H15O4P · C2H4O · O5P2)n
Phosphorous content	19% (Fyrol PNX and Fyrol PNX-LE; Aflammit PLF 140)
Abbreviation, synonyms	Phosphoric acid, triethyl ester, polymer with oxirane and phosphorus oxide (P2O5)
FR products and manufacturers	Fyrol PNX (ICL-IP Europe) Fyrol PNX-LE (ICL-IP Europe) Aflammit PLF 140 (THOR)
Registered tonnage, t/year	Pre-registered
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Flexible and rigid polyurethane foams, cellulosic plastic composite
End applications	Flexible foams in automotive, bedding and seating
Reactive/additive	Indicated as both additive and reactive
Health env. profiles	PUR, US EPA, 2015
Availability	This FR and FRs with similar chemistry are available from several manufacturers
Flame retardancy	It is indicated that the flame retardants is most suitable for MVSS 302 (motor vehicle standard) and Cal 117 type foams (California standard for resilient filling materials), but also applicable in UL94HF foams (for EEE). Its high molecular weight is another advantage in automotive foams because in suitable formulations it is low fogging and can give foams low in VOC emissions, passing the general automotive volatile requirements. No data on market penetration has been obtained. (Lassen et al., 2015)
Halogen-containing	TCPP, TDCP

flame retardants for the same application (examples)	

Hazard profile

The screening of oligomeric ethyl ethylene phosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 24
SCORING OF OLIGOMERIC ETHYL ETHYLENE PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	M	L	L	DG	**L**	DG	L	DG	M	L	DG	**L**	**M**	**L**	L	**VH**	L	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

Limited data were available for the substance. The scores for carcinogenicity, genotoxicity, reproductive and developmental effects provided by the US EPA are based on estimations and expert judgement, the latter also taking the polymer's limited bioavailability and structural alerts into account.

The persistence designation "very high" for the polymer is based on experimental data and professional judgement for its higher MW components (MW >1,000).

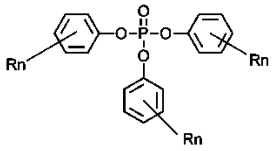
Overall hazard scoring

An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1, but meets criterion c) for Benchmark 2 by scoring "high" for persistence and "moderate" for carcinogenicity and irritation of the eye.

4.4 Organophosphates (phosphate esters) – Aryl alkyl phosphates

4.4.1 Isopropyl phenyl phosphate, CAS No. 68937-41-7

Technical description

CAS No	68937-41-7		
EC No	273-066-3		
Chemical name	Isopropyl phenyl phosphate		
Structural formula	 R = isopropyl; n = 0, 1, 2 or 3 Registration		
General formula			
Phosphorous content	8.3% (Phosflex 31L/41L; EVERFOS 1500; Reofos® 50; Reofos® 65) 8.6% (EVERFOS 1350; Reofos® 35) 8.1% (EVERFOS 1650) 7.6% (EVERFOS 1950) 7.5% (EVERFOS 4000)		
Abbreviation, synonyms	Phenol, isopropylated, phosphate (3:1), IPPP; ITP; IPTPP; TIPPP; Isopropylated triphenyl phosphate; Isopropylated phenol phosphate		
FR products and manufacturers	EVERFOS 1350, EVERFOS 1500, EVERFOS 1650, EVERFOS 1950, EVERFOS 4000 (Everkem) Reofos® 35, Reofos® 50, Reofos® 65, Reofos® 95 (Great lake solutions) Phosflex 31L, Phosflex 41L (ICL-IP Europe)		
Registered tonnage, t/year	10,000 – 100,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid thermoplastics	PC/ABS	Applicable
		HIPS/PPO	Applicable
	Foams	PUR flexible foam	Applicable
		PVC/nitrile foam	Applicable
		Rubbers/elastomers	Applicable
	Textile/paints/adhesives	Hot melts	Applicable
		Paints	Applicable
		Latex/adhesives	Applicable
	Thermosets	Phenolic resins	Applicable
	Wires and cables	PVC flexible	Applicable
		TPU	Applicable
Other information on substrate	PVC, cellulosic resins, and synthetic rubber, EPDM, HIPS, PC/ABS (alloys), PPO/HIPS (alloys), rigid and flexible polyurethane, TPU, epoxyresin, phenolics resin, PC, Coating (paint), textile (back coating), adhesive, rubbers.		
End applications	-		
Reactive/additive	Additive		
Health env. profiles	Flame retardants used in flexible polyurethane foam (US EPA, 2015).		
Availability	Availalable from many manufacturers, widely used for many years.		

Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	TCCP, DBDPE; EBTEBPI

Hazard profile

The screening of isopropylated triphenyl phosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 25
SCORING OF ISOPROPYLATED TRIPHENYL PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	H	M	DG	L	DG	H	H	H	L	DG	L	L	VH	VH	M	VH	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

Commercial products of the alternative isopropylated triphenyl phosphate may contain a mixture consisting of isopropylated triphenyl phosphates with an unspecified degree of isopropylation. Therefore tris(isopropylphenyl) phosphate isomers and other related compounds have been included in the assessment.

Due to lack of data, the US EPA assesses the carcinogenic potential as uncertain and assigns the "moderate" score to this endpoint. Based on weight of evidence including negative results in gene mutation tests, mutagenicity/genotoxicity was scored as low.

The scores for reproductive, developmental, systemic and neuro-toxicity are based on experimental data. Furthermore, the potential for neurotoxicity is supported by the structural alert for organophosphates.

With respect to endocrine activity, no data were available for this substance. However, tests with commercial products containing analogues (components not further specified) indicate endocrine activity, but it is unclear which component or components of the mixture are driving the endocrine activity effects. We therefore mark this endpoint as data gap.

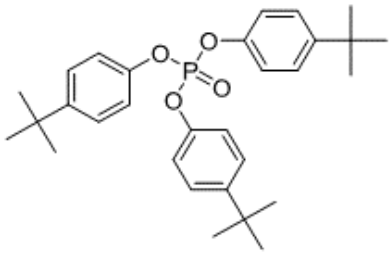
Numerous experimental studies, supported by QSAR estimations, lead to the "very high" scores for aquatic toxicity. Experimental studies with commercial products are also available for persistence and bioaccumulation. Nonetheless, the bioaccumulation designation "High" in the US EPA report is based on the estimated BAF values (estimations for representative structures for components of the mixture) being >1,000, and two of the six estimated values do also exceed 5000. The US EPA states lower confidence in the experimental BCF values because they are not consistent with the limited water solubility of the substances and because the studies were performed on commercial products consisting of mixtures of unquantified components. Using a conservative approach and considering

adequate measured log Kow values (4.92 to 5.17) for commercial products, we have assigned the score “very high” based on the estimated BAF values.

Overall hazard scoring
An overall hazard score = 1 has been assigned because the substance scores “Very high” for the endpoints acute and chronic aquatic toxicity, as well as for bioaccumulation, thus fulfilling criterion d) of Benchmark 1. Furthermore, the substance scores “High” for Group I and II* Human.

4.4.2 Tris (p-t-butylphenyl) phosphate, CAS No. 78-33-1

Technical description

CAS No	78-33-1
EC No	201-106-1
Chemical name	Tris (p-t-butylphenyl) phosphate
Structural formula	 US EPA, 2015
General formula	C30H39O4P
Phosphorous content	
Abbreviation, synonyms	Phenol, 4-(1,1-dimethylethyl)-, 1,1`,1``-phosphate
FR products and manufacturers	Part of Phosflex 71B (ICL-IP Europe)
Registered tonnage, t/year	Not registered
Pinfa Product Selector	Not in PPS
Other information on substrate	HIPS/PPO, PC/PC ABS, flexible PVC
End applications	PVC & textile adhesive coatings
Reactive/additive	Additive
Health env. profiles	Flame retardants used in flexible polyurethane foam (US EPA, 2015).
Availability	-
Flame retardancy	UL94 V0/V1 grades of HIPS/PPO and PC/ABS
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile
The screening of tris (p-t-butylphenyl) phosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 26
SCORING OF TRIS (P-T-BUTYLPHENYL) PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	M	L	DG	L	DG	H	DG	M	M	DG	M	L	VH	VH	M	H	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
Commercial products of the alternative TBPP may contain a mixture of t-butyl isomers and t-butyl substituted phenyl phosphate esters depending on the manufacturing, purification and processing of the compound. TBPP isomers and t-butyl substituted phenyl phosphate esters are anticipated to be present in commercial products and were therefore considered in the evaluation by the US EPA.

Due to lack of data, the US EPA assesses the carcinogenic potential as uncertain and assigns the score "moderate" score to this endpoint. Based on experimental studies yielding negative results in gene mutation tests, mutagenicity/genotoxicity was scored as low.

The scores for reproductive, developmental, systemic and neuro-toxicity are based on experimental data with mixture components of TBPP and in a few cases (reproductive and repeated dose effects) also individual isomers of TBPP.

With respect to endocrine activity, no data were available for this test substance. Tests with related compounds (hydraulic BTP: mixture of p-t-butylphenyl phenyl phosphates (84%), triphenyl phosphate, and m-t-phenyl phosphate), demonstrated changes in adrenal glands and ovaries. These test are, however, not sufficient for applying a score to this endpoint, we therefore mark endocrine activity as data gap.

Experimental data for mixture components of TBPP are available for skin sensitization and irritation of skin and eye, but no data are available for respiratory sensitization.

The hazard designations for aquatic toxicity are based on experimental data for mixture components of TBPP for fish and daphnia.

The persistence designation is derived from measured values for t-butylphenyl diphenyl phosphate (CASRN 56803-37-3). For the same substance, measured bioaccumulation values are available from non-guideline studies, which are used by the US EPA for hazard designation. The QSAR-estimated BAF for tris (p-t-butylphenyl) phosphate is 100,000, even though the authors note that the value may be overestimated given the limited water solubility. Using a conservative approach and considering measured and estimated log Kow values > 5, we have assigned the score "very high" based on the estimated BAF value.

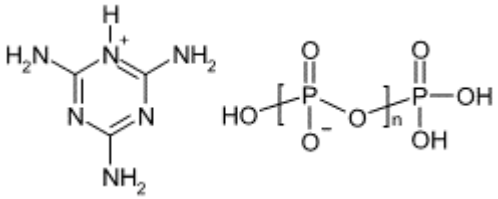
Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1. The overall hazard 2 criterion f) requires only "very high" (Ecotoxicity,

Group I, II or II* Human), while the substance also scores “high” in B and Group II and II* Human. Thus, the Benchmark score 2 does not fully reflect the hazard potential of the substance.

4.5 Melamine-derived and other organic phosphates (not being esters)

4.5.1 Melamine pyrophosphate, CAS No. 15541-60-3

Technical description

CAS No	15541-60-3
EC No	239-590-1
Chemical name	Melamine pyrophosphate
Structural formula	 US EPA, 2014a
General formula	C3H10N6O7P2
Phosphorous content	>14% (Everflam MPP-2)
Abbreviation, synonyms	Melamine polyphosphate (US EPA 2014a) diphosphoric acid, compound with 1,3,5-triazine-2,4,6-triamine
FR products and manufacturers	EVERFLAM MPP-2 (Everkem) AFLAMMIT® PMN 370 (THOR)
Registered tonnage, t/year	Pre-registered
Pinfa Product Selector	Not Coating (paint), textile (back coating)identified in PPS
Other information on substrate	Various fabrics, nylons, paints, paper and plastics; mainly used for coating/paint and textile backcoating (Everkem)
End applications	-
Reactive/additive	Additive
Health env. profiles	Alternatives to decaBDE (US EPA, 2014a)
Availability	-
Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	HBCDD

Hazard profile

The screening of melamine phosphate by the modified GreenScreen® methodology was based on information compiled according to the information sources described in 3.2.1.

TABLE 27
SCORING OF MELAMINE PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	DG	L	L	VH	VL	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
Experimental studies with melamine phosphate are sparse. Therefore, the hazard designations are based on studies performed with melamine. The only exceptions are genotoxicity assays performed with melamine phosphate.

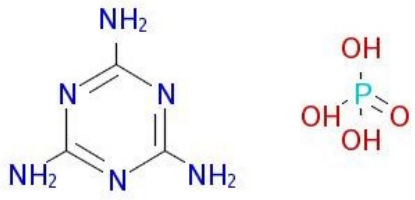
There is experimental evidence that oral melamine exposure causes carcinogenicity in animals; however, no data were located to support its carcinogenicity in humans. The experimental results on melamine, in accordance with the scoring of melamine polyphosphate (section 4.5.1), justify the moderate score. Genotoxicity tests with melamine phosphate yielded negative results.

Experimental data on reproductive and developmental effects of melamine phosphate were not available. However, corresponding to the scoring of melamine polyphosphate (section 3.5.4) and read-across with melamine, a low hazard is assigned to these endpoints.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1, but meets criterion c) for Benchmark 2 by scoring "very high" for persistence (only "high" is required for Benchmark 2) and "moderate" for carcinogenicity and systemic toxicity.

4.5.2 Melamine phosphate, CAS No. 41583-09-9

Technical description

CAS No	41583-09-9
EC No	255-449-7
Chemical name	1,3,5-triazine-2,4,6-triamine phosphate (pre-registration)
Structural formula	 REACH Registration data
General formula	C3H6N6.xH3O4P
Phosphorous content	10 - 13% (MPT11)
Abbreviation, synonyms	Melamine phosphate, reaction product of 1,3,5-triazine-2,4,6-triamine phosphate and orthophosphoric acid
FR products and manufacturers	Melapur MP (BASF) Melagard MP (Italmatch) MPT11 (Metadynea Austria GmbH) AFLAMMIT® PMN 185 (THOR) Budit 312 (Budenheim)
Registered tonnage, t/year	1,000 - 10,000
Pinfa Product Selector	Group: / Substrate: / Applicability: Solid Thermoplastics / Polyethylene (PE) / Applicable Solid Thermoplastics / Polypropylene (PP) / Applicable Textiles/Paints/Adhesives / Paints / Applicable Textiles/Paints/Adhesives / Intumescent Coatings / Applicable Textiles/Paints/Adhesives / Textile backcoating / Applicable Thermosets / Unsaturated polyesters / Applicable Thermosets / Phenolic Resins / Applicable Thermosets / Epoxy Resins / Applicable
Other information on substrate	Thermoplastics, polyolefins, elastomers, engineering resins, paints, intumescent fire retardant coating.
End applications	-
Reactive/additive	Reactive
Health env. profiles	Screened as part of this study (see below)
Availability	Available for many years from many manufacturers
Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile

The screening of melamine phosphate by the modified GreenScreen® methodology was based on information compiled according to the information sources described in 3.2.1. The full data set from the data collection including justification of the scoring is enclosed as Appendix 7 to this report.

TABLE 28
SCORING OF MELAMINE PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	DG	L	L	VH	VL	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

Experimental studies with melamine phosphate are sparse. Therefore, the hazard designations are based on studies performed with melamine. The only exceptions are genotoxicity assays performed with melamine phosphate.

There is experimental evidence that oral melamine exposure causes carcinogenicity in animals; however, no data were located to support its carcinogenicity in humans. The experimental results on melamine, in accordance with the scoring of melamine polyphosphate (section 4.5.1), justify the moderate score. Genotoxicity tests with melamine phosphate yielded negative results.

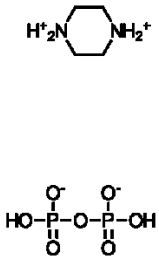
Experimental data on reproductive and developmental effects of melamine phosphate were not available. However, corresponding to the scoring of melamine polyphosphate (section 3.5.4) and read-across with melamine, a low hazard is assigned to these endpoints.

Overall hazard scoring

An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1, but meets criterion c) for Benchmark 2 by scoring “very high” for persistence (only “high” is required for Benchmark 2) and “moderate” for carcinogenicity and systemic toxicity.

4.5.3 Diphosphoric acid, compd. with piperazine, CAS No. 66034-17-1, and substituted amine phosphate (confidential CAS No.)

Technical description

CAS No	66034-17-1		
EC No	457-330-7		
Chemical name	Diphosphoric acid, compd. with piperazine		
Structural formula	 Registration		
General formula	Not available		
Phosphorous content	55-65% (ADK STAB FP-2100J) 16-21% ADK STAB FP2200)		
Abbreviation, synonyms			
FR products and manufacturers	ADK STAB FP-2100J, ADK STAB FP-2200 (Adeka Palmarole)		
Registered tonnage, t/year	10 – 100		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	Polypropylene (PP)	Applicable
		Polyethylene (PE)	Applicable
		Thermoplastic elastomers	Applicable
		EVA-cop.	Applicable
	Foams	Rubbers/Elastomers	Could be applied
	Textiles/Paints/Adhesives	Textile backcoating	Could be applied
		Intumescent Coatings	Applicable
		Latex/adhesives	Could be applied
		Hot melts	Could be applied
	Thermosets	Epoxy Resins	Could be applied
		Unsaturated polyesters	Applicable
		Vinyl esters	Could be applied
		Acrylic resins	Could be applied
	Wire and cables	TPU	Applicable
		Polypropylene (PP)	Applicable
		EPDM	Applicable
		PE/EVA	Applicable
Other information on substrate	-		
End applications	-		

Reactive/additive	Additive
Health env. profiles	Alternatives for the flame retardant decaBDE (US EPA, 2014a)
Availability	-
Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile

The screening of the piperazine pyrophosphate and the substituted amine phosphate (confidential CAS no.) by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 29
SCORING OF DIPHOSPHORIC ACID, COMPD. WITH PIPERAZINE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	M	M	M	DG	H	DG	M	DG	DG	**L**	M	**L**	**M**	M	L	H	L	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

Piperazine pyrophosphate constitutes approximately 50% of the commercial mixtures. The remaining 50% are made of a confidential substituted amine phosphate. For most endpoints, experimental studies on both piperazine and the substituted amine phosphate component are available.

The US EPA estimates the carcinogenicity hazard potential as moderate based several animal studies with the substituted amine phosphate component. Positives results in *in vitro* and *in vivo* studies with the substituted amine phosphate component lead to the conclusion on moderate mutagenicity/genotoxicity. Based on data for the piperazine moiety, the reproductive hazard potential was estimated to be moderate. Based on data for the piperazine moiety and professional judgement, the hazard potential for developmental effects and respiratory sensitization were likewise estimated to be moderate. With respect to neurotoxicity, no data were available.

In the only study available on endocrine activity, the substituted amine phosphate component did not exhibit estrogenic activity *in vitro* assay. The data are insufficient for an evaluation, we therefore mark the endpoint as DG (data gap).

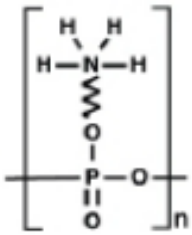
Regarding persistence in the environment, the substituted amine phosphate mixture is estimated to show high persistence based on experimental data for the organic components. Low potential for bioaccumulation was based on both QSAR estimations and a confidential study of the amine phosphate component.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1. However, the Benchmark 2 criterion c) only requires "high" P and "moderate" T (Ecotoxicity, Group I, II or II* Human), while the substance scores "high" in P and T.

4.6 Inorganic phosphorous compounds

4.6.1 Ammonium polyphosphate, CAS No. 68333-79-9

Technical description

CAS No	68333-79-9
EC No	269-789-9
Chemical name	Ammonium polyphosphate
Structural formula	 Everkem product catalogue
General formula	NH_4PO_3
Phosphorous content	12.5-13.5% (Exolit® AP 420) 17-19% (Exolit® AP 740 S) 18-20% (Exolit® AP 740 F, Exolit® AP 740) 19-21% (Exolit® AP 760) Approx. 20% (Exolit® AP 755) 20-22% (Exolit® AP 750) 21-23% (Exolit® AP 742) 23-25% (Exolit® AP 765 (TP), Exolit® AP 766 (TP)) 29-31% (Exolit® AP 462, Preniphor EPFR-APP241, Preniphor EPFR-APP262) 29.5-31.5% (Preniphor EPFR-APP231) 31-32% (Exolit® AP 423, Exolit® AP 422, EVERFLAM APP, Preniphor EPFR-APP222H, Preniphor EPFR-APP222, Preniphor EPFR-APP223, Preniphor EPFR-APP224, Preniphor EPFR-APP263)
Abbreviation, synonyms	APP; Ammonium polyphosphate (with synergists); Ammonium polyphosphate (coated); Polyphosphoric acids, ammonium salts
FR products and manufacturers	BUDIT 3123, BUDIT 3167, BUDIT 3168, BUDIT 3178, FR CROS 484, FR CROS C30, FR CROS C60, (Budenheim). Exolit® AP 740 F, Exolit® AP 462, Exolit® AP 423, Exolit® AP 742, Exolit® AP 750, Exolit® AP 422 , Exolit® AP 420, Exolit® AP 760, Exolit® AP 755, Exolit® AP 740 , Exolit® AP 740 S, Exolit® AP 765 (TP), Exolit® AP 766 (TP), (Clariant) EVERFLAM APP (Everkem) AFLAMMIT® PCI 202 (Thor) Preniphor EPFR-APP222H, Preniphor EPFR-APP222, Preniphor EPFR-APP223, Preniphor EPFR-APP224, Preniphor EPFR-APP231, Preniphor EPFR-APP241, Preniphor EPFR-APP262, Preniphor EPFR-APP263, (Presafer) Mileflame NP 1000 (MPI Chemie BV)

	Other product based on ammonium polyphosphate Phos-Chek ® LC95W Solution Phos-Chek ® LC95W FT936 / Fire-Trol 936 FT934 / Fire-Trol 934 FT931 / Fire-Trol 931 Phos-Chek ® LC95A-F BUDIT® IS 3001 AFLAMMIT® PPN series		
Registered tonnage, t/year	10,000 - 100,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	Polypropylene (PP)	Applicable
		Polyethylene (PE)	Applicable
		Thermoplastic elasto-mers	Could be applied
		EVA-cop.	Applicable
	Foams	Rubbers/Elastomers	Could be applied
		PUR flexible foam	Applicable
		PUR Rigid foam	Applicable
	Textiles/Paints/Adhesives	Other textile fibres	Applicable
		Intumescent Coatings	Applicable
		Hot melts	Could be applied
		Latex/adhesives	Could be applied
		Textile backcoating	Could be applied
	Thermosets	Acrylic resins	Applicable
		Epoxy Resins	Applicable
		Phenolic Resins	Applicable
		Unsaturated polyes-ters	Applicable
		Vinyl esters	Could be applied
	Wire and cables	PE/EVA	Applicable
	Others	Paper/Wood	Could be applied
Other information on substrate	Unsaturated polyester resin, acrylic resins, epoxy or phenolics. PP, PE, PP copolymers and PP blends. Rigid and flexible polyurethane, TPU, epoxy resin, coating (paint)		
End applications	Building materials/Construction, transportation, EEE, furniture, wood, pa-per, textiles, intumescent coatings		
Reactive/additive	Additive		
Health env. profiles	Flame retardants used in flexible polyurethane foam (US EPA, 2015).		
Availability	Have been available for many years from many manufacturers		
Flame retardancy	V-0 grade PP and PE for EEE can be obtained by loadings of 26-30% and 30-35%, respectively, ammonium polyphosphate (Lassen et al., 2006) Alternative for decaBDE for natural synthetic fibres (Illinois EPA, 2007)		
Halogen-containing flame retardants for the same application (ex-amples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others		

Hazard profile

The screening of ammonium polyphosphate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 30
SCORING OF AMMONIUM POLYPHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	L	L	L	**L**	L	L	L	L	**L**	DG	**L**	**L**	**L**	L	**(VH)**	L	4

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

No experimental data were located with respect to carcinogenicity, mutagenicity/genotoxicity, reproductive and developmental effects, endocrine activity, repeated dose effects and neurotoxicity. Therefore, professional judgement considering the polymer´s molecular weight (MW >1,000) and limited bioavailability justify the scoring of these endpoints.

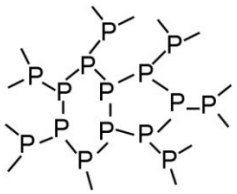
Several experimental studies are listed in the US EPA report concerning the endpoints acute aquatic toxicity and persistence. Furthermore, these endpoints as well as chronic aquatic toxicity and bioaccumulation are characterized by QSAR estimates.

Overall hazard scoring

The substance scores “low” for all endpoints, apart from persistence. However, since the substance is inorganic and persistence is not combined with chronic effects, a Benchmark 4 can be assigned.

4.6.2 Red phosphorus, CAS No. 7723-14-0

Technical description

CAS No	7723-14-0		
EC No	918-594-3		
Chemical name	Red phosphorus		
Structural formula	 Registration		
General formula	Not available		
Phosphorous content	43.0 - 48.0% (Exolit® RP 6520) 60.0 - 63.0% (Red Phosphorus PU 6580, Exolit® RP 607) 50% (MASTERET 70450, MASTERET 80450, MASTERET 20450) 60% (MASTERET 10460 B2XF, MASTERET 15460 B2XF, MASTERET 40460 B2XF, MASTERET 63460 B2XF) 70% (MASTERET 10170) >90% (Exolit® RP 614 presscake (TP) >95.0% (Red Phosphorus HB 801)		
Abbreviation, synonyms	Red phosphorus, concentrates; Red phosphorus, dispersions		
FR products and manufacturers	Red Phosphorus HB 801, Red Phosphorus PU 6580, Exolit® RP 607, Exolit® RP 6520, Exolit® RP 614 presscake (TP), (Clariant) MASTERET 10170, MASTERET 63460 B2XF, MASTERET 70450, MASTERET 10460 B2XF, MASTERET 15460 B2XF, MASTERET 20450, MASTERET 40460 B2XF, MASTERET 80450 (Italmatch)		
Registered tonnage, t/year	1,000 - 10,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	Polyamide (PA)	Applicable
		Polypropylene (PP)	Could be applied
		Polyethylene (PE)	Could be applied
	Foams	Rubbers/Elastomers	Could be applied
		PUR Rigid foam	Applicable
	Thermosets	Epoxy Resins	Applicable
		Unsaturated polyesters	Could be applied
		Phenolic Resins	Could be applied
	Textiles/Paints/Adhesives	Hot melts	Could be applied
		Latex/adhesives	Applicable
		Other textile fibres	Applicable
Other information on substrate	Solid plastics, closed cell foams, polymer adhesives, polyisocyanurate and polyurethane rigid foams, plastics, polyurethanes, synthetic and natural rubber latex systems, polyolefines articles, epoxy resins, polypropylene articles and sometimes in PA.		
End applications	EEE, automotive applications		

Reactive/additive	Additive
Health env. profiles	Alternatives for decaBDE (US EPA, 2014a)
Availability	Available from many manufacturers. Account for a significant share of flame retarded polyamide in EEE (Lassen et al., 2006)
Flame retardancy	Vo grade glass reinforced polyamide (PA 66) for use in electrical and electronic equipment can be obtained with loadings of 10-13% red phosphorus (Lassen et al., 2006) Can be used for electronics applications and must be combined with aluminium hydroxide (Morose, 2006).
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile

The screening of Red phosphorus by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decaBDE (US EPA, 2014a).

TABLE 31
SCORING OF RED PHOSPHORUS USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	**M**	L	L	DG	**L**	L	L	L	L	**L**	DG	**M**	**M**	L	L	**H**	L	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

The evaluation of carcinogenicity and reproductive effects is based on expert judgement. A single secondary source indicates weak mutagenic effects, due to uncertainty about this endpoint, the US EPA designates the score “moderate”. The evaluation of reproductive and developmental effects, systemic toxicity as well as neurotoxicity is based in expert judgement.

The authors of the report also refer to several animal studies on exposure to a pyrotechnic mixture containing red phosphorous (red phosphorus/butyl rubber aerosols or smoke), demonstrating immunotoxic, lethal and repeated dose effects. However, the toxicity reported could, according to the authors’ evaluation, not be attributed to any of the components of the mixture including red phosphorus.

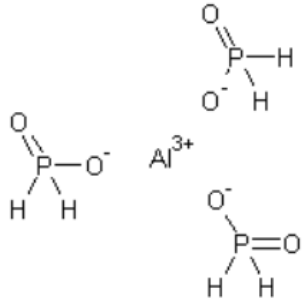
With respect to aquatic toxicity, several studies report effects at concentrations above the water solubility limit. Therefore, no effects at saturation can be assigned.

Overall hazard scoring

An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1, but meets criterion c) for Benchmark 2 by scoring "high" for persistence and moderate” for mutagenicity/genotoxicity as well as eye sensitization and irritation.

4.6.3 Phosphinic acid, aluminium salt (3:1), CAS no. 7784-22-7

Technical description

CAS No	7784-22-7
Chemical name	Phosphinic acid, aluminium salt (3:1)
Structural formula	 Registration data
General formula	-
Phosphorous content	-
Abbreviation, synonyms	Hypophosphite, aluminium salt
FR products and manufacturers	Phoslite IP-A (Italmatch)
Registered tonnage, t/year	10 - 100
Pinfa Product Selector	With synergist: **Group:** / **Substrate:** / **Applicability**: Solid Thermoplastics / PBT / applicable Polyamide (PA) / applicable Polypropylene (PP) / applicable Thermoplastic elastomers / applicable Foams / XPS foam / applicable Polypropylene foam (PP) / applicable Rubbers/Elastomers / applicable Textiles/Paints/Adhesives / Other textile fibres / applicable Thermosets / Epoxy Resins / applicable Unsaturated polyesters / applicable Wire and cables / PVC flexible / applicable Polypropylene (PP) / applicable TPU / applicable PE/EVA / applicable
Other information on substrate	It is a new family of white products intended to be used in polypropylene (PP) as well as in engineering polymers, in particular in polyamides, PBT, PC and PC Alloys, but also as antimony trioxide replacement (Italmatch)
End applications	-
Reactive/additive	Additive
Health env. profiles	Screened as part of this study
Availability	Recently introduced line of FR additives (Italmatch)
Flame retardancy	Intended for polypropylene (PP) UL 94 V2 applications, PBT UL 94 V0, ABS, PVC, PC and PC Alloys
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile

The screening of this alternative by the modified GreenScreen® methodology was based on information compiled according to the information sources described in 3.2.1. The full data set from the data collection including justification of the scoring is enclosed as Appendix 6 to this report.

TABLE 32
SCORING OF PHOSPHINIC ACID, ALUMINIUM SALT (3:1) USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
DG	L	L	L	DG	L	DG	M	DG	DG	L	DG	L	M	M	M	(VH)	L	3

Comments to hazard profile scores

Apart from the REACH registration data, no other data sources provide information on the substance. QSAR estimations are not applicable, because the substance is inorganic. Most of the scores, for which experimental data were available, are based on studies with a commercial product.

No studies were available for persistence and bioaccumulation, the scores of these endpoints are therefore based on read-across and professional judgement. Since the substance is inorganic, persistence is not considered a negative characteristic.

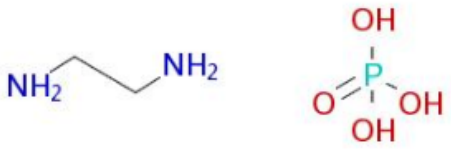
Overall hazard scoring

An overall hazard score = 3 has been assigned, even though the substance formally fulfils the criterion c) for Benchmark 2 by scoring “very high” for persistence (only “high” required for Benchmark 2) and “moderate” for several toxicity endpoints. However, the persistence score is exempted from the evaluation because the substance is inorganic. Thus criteria b) and c) behind overall hazard 3 are fulfilled (“moderate ecotoxicity” and “moderate T”, respectively).

4.7 Other phosphorous and non-categorised substances

4.7.1 Ethylenediamine-o-phosphate, CAS No. 14852-17-6

Technical description

CAS No	14852-17-6
EC No	238-914-9
Chemical name	ethylenediamine, salt with phosphoric acid
Structural formula	 Reach registration data
General formula	C2H8N2.xH3O4P
Phosphorous content	18 – 21 (Metadynea, 2014)
Abbreviation, synonyms	EDAP, EP11
FR products and manufacturers	EP11 (Metadynea Austria GmbH) Aflammit® PCO 123/234 (THOR)
Registered tonnage, t/year	0 - 10
Pinfa Product Selector	Group: Substrate: Applicability: Solid Thermoplastics Polyethylene (PE) Applicable Polypropylene (PP) Applicable EVA-cop. Applicable Textiles/Paints/Adhesives Paints Applicable Intumescent Coatings Applicable Hot melts Could be applied Textile backcoating Applicable Thermosets Epoxy Resins Could be applied Unsaturated polyesters Could be applied
Other information on substrate	Solid Thermoplastics
End applications	Recommended for electronics and electricals, transportation, construction.(Thor)
Reactive/additive	Additive
Health env. profiles	Screened as part of this study (see below)
Availability	-
Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile

The screening of this alternative by the modified GreenScreen® methodology was based on information compiled according to the information sources described in 3.2.1. The full data set from the data collection including justification of the scoring is enclosed as Appendix 8 to this report.

TABLE 33
SCORING OF ETHYLENEDIAMINE PHOSPHATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	L	M	DG	L	DG	M	DG	DG	H	H	VH	L	M	H	VL	VL	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
Ethylenediamine phosphate (CAS No. 14852-17-6) consist of a mixture of ethylenediamine and phosphoric acid. Only very limited data are available for ethylenediamine phosphate. Ethylenediamine (CAS No. 107-15-3) is therefore used as chemical surrogate in case of lack of data for ethylenediamine phosphate.

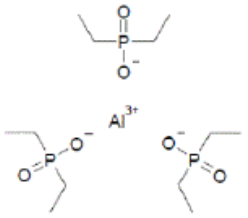
Ethylenediamine has a harmonised classification comprising the following health hazards: Acute Tox. 4 * (H302), Acute Tox. 4 * (H312), Skin Corr. 1B (H314), Skin Sens. 1 (H317), Resp. Sens. 1 (H334). Phosphoric acid (CAS No. 7664-38-2) also has a harmonised classification: Skin Corr. 1B (H314).

The human endpoints carcinogenicity, developmental and systemic toxicity as well as respiratory sensitization and dermal irritation are based read-across on data for ethylenediammonium dichloride, ethylenediamine and/or QSAR estimates. The same applies to the aquatic toxicity and fate endpoints.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1, but meets criterion e) and f) for Benchmark 2 by scoring “Moderate” for developmental toxicity (Group I Human) and “ Very high” and “High” for other endpoints in Group II Human and ecotoxicity.

4.7.2 Diethylphosphinate, aluminium salt, CAS No. 225789-38-8

Technical description

CAS No	225789-38-8		
EC No	*607-114-5		
Chemical name	Diethylphosphinate, aluminium salt		
Structural formula	 US EPA 2014b		
General formula	3 C4H11PO2·Al		
Phosphorous content	*Neat Al-diethylphosphinates:* 23.3 - 24.0% (Exolit® OP 930, Exolit® OP 935, Exolit® OP 1230, Exolit® OP 1240) Blends of Al-diethylphosphinate with one or more other substances (e.g. melamine polyphosphate (synergist)): 18.7 - 19.7% (Exolit® OP 1312) 19.7 - 20.7% (Exolit® OP 1311) 19.8 - 20.8% (Exolit® OP 1260 (TP)) 20.5 - 21.5% (Exolit® OP 1314) 24.5 - 25.5% (Exolit® OP 1400)		
Abbreviation, synonyms	Phosphinic acid, P,P-diethyl-, aluminium salt (3:1)		
FR products and manufacturers	Exolit® OP 930, Exolit® OP 935, Exolit® OP 1230, Exolit® OP 1240, Exolit® OP 1260 (TP), Exolit® OP 1311, Exolit® OP 1312, Exolit® OP 1314, Exolit® OP 1400 (Clariant)		
Registered tonnage, t/y	Pre-registered		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	Thermoplastic elastomers	Could be applied
		Polyamide (PA)	Could be applied
		PBT	Applicable
		PET	Applicable
	Textiles/Paints/Adhesives	Other textile fibres	Could be applied
	Thermosets	Acrylic resins	Could be applied
		Epoxy resins	Applicable
	Wire and cables	TPU	Applicable
Other information on substrate	High temperature polyamides , polyesters, reinforced polyamide (6 and 66)		
End applications	EEE, automotive		
Reactive/additive	Additive		
Health env. profiles	Alternatives to the halogenated flame retardant in printed circuit boards (US EPA, 2014b)		
Availability	Have been on the marked for many years. Have mainly been applied for epoxy		

	resins, TBU and PBT/PET
Flame retardancy	Vo grade PBT for EEE can be obtained with loadings of about Exolit® OP 1312 while Vo grade PA can be obtained with loadings of 15-20% (Lassen et al., 2006) Aluminium diethyl phosphinates were originally developed for glass-fibre reinforced polyamides and polyester achieved UL 94-Vo rating in with ~40 wt % additive (Rakotamala, 2010). Vo grade phenol novolac epoxy resin can be obtained with about 10% aluminium diethylphosphinate-based flame retardants (Rakotamala, 2010) (other loadings in combination with other flame retardants). UL 94-Vo rating could be achieved with a combined flame retardant loading of 20 wt % aluminium diethylphosphinate and melamine cyanurate (Rakotamala, 2010). It has been reported that metal phosphinates are most effective in combination with a nitrogen synergist, such as melamine polyphosphate (Rakotamala, 2010).
Halogen-containing flame retardants for the same application (examples)	TBBPA (reactive and additive), decaBDE

Hazard profile

The screening of Aluminium Diethylphosphinate by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives to the halogenated flame retardant in printed circuit boards (US EPA, 2014b).

TABLE 34
SCORING OF ALUMINIUM DIETHYLPHOSPHINATE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
L	L	L	M	DG	L	M	M	DG	M	L	DG	L	L	M	M	H	L	2

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores

Aluminium diethylphosphinate is estimated to be of low hazard for carcinogenicity based on comparison to analogous metal salts and professional judgement. The US EPA estimates the substance to be of moderate hazard for immunotoxicity due to the presence of a bioavailable aluminium and based on comparison to analogous metal salts and professional judgement.

According to professional judgement, neurodevelopmental effects may occur due to the presence of a phosphinate. Experimental studies specifically designed to evaluate the neurodevelopmental endpoint were not located, and the single available developmental toxicity screening study available did not show any adverse effects. Based on a conservative approach, the assessment by the US EPA is shared here. Aluminium diethylphosphinate is scored to be of "moderate" hazard for neurotoxicity based on analogy to aluminium hydroxide and professional judgement.

Estimates for the organic counter-ion indicate that the half-life for ultimate aerobic biodegradation in water is less than 60 days, corresponding to the moderate potential for persistence. The metal ion is recalcitrant to biodegradation or other typical environmental removal processes, resulting in a "High" score for persistence.

Overall hazard scoring
An overall hazard score = 2 has been assigned because the substance does not fulfil any of the criteria behind Benchmark 1 but meets criterion e) for Benchmark 2 by scoring "moderate" for toxicity in Group I.

4.7.3 Confidential halogen-free flame retardant, Emerald Innovation™ NH-1*

Technical description

CAS No	Confidential
EC No	-
Chemical name	Confidential
Structural formula	N.a.
General formula	N.a.
Phosphorous content	7.9 % (Emerald Innovation™ NH-1)
Abbreviation, synonyms	-
FR products and manufacturers	Emerald Innovation™ NH-1 (Great Lake Solutions)
Registered tonnage, t/year	-
Pinfa Product Selector	Not identified in PSS
Other information on substrate	Flexible Polyurethane foams
End applications	"Is an effective, halogen-free replacement for chlorinated phosphate esters in furniture and automotive flexible polyurethane foam applications" (Great Lake Solutions)
Reactive/additive	Additive
Health env. profiles	Flame retardants used in flexible polyurethane foam (US EPA, 2015)
Availability	-
Flame retardancy	Effective in meeting a variety of fire safety standards, including British Standard 5852 Crib V, California Technical Bulletin 117, FMVSS 302 and UL94 HF-1 (Great Lake Solutions)
Halogen-containing flame retardants for the same application (examples)	TCCP, TDCP

Hazard profile
The screening of this confidential flame retardant by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 35
SCORING OF THE CONFIDENTIAL HALOGEN-FREE FLAME RETARDANT USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	M	L	H	H	DG	H	DG	M	M	DG	M	M	VH	VH	M	H	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
The confidential flame retardant Emerald Innovation™ NH-1* consists of 3 components (Confidential C, Confidential D and Confidential E), all with confidential CAS No. Experimental and measured data for the single compounds are listed in the US EPA report (2015), but are summarized in one hazard table here.

Carcinogenic effects cannot be ruled out, because there is uncertainty due to lack of data for Confidential C and E. A “moderate” hazard has been designated for reproductive effects based on uncertainty due to lack of more definite studies on Confidential C.

The designations for the other human endpoints are based on experimental data for the confidential components C, D, and E.

With respect to endocrine activity, studies were available for two of the components. Component D showed endocrine activity in some *in vitro* assays, impaired reproduction in zebra fish and a single study also suggests human health effects (decreased sperm count and altered hormone levels in men) related to exposure of component D. The actual exposure to component D is, however, unknown in the latter study. Based on a conservative approach, we assign the score "High" to the endpoint of endocrine activity.

Experimental data for component D and E trigger a “very high” hazard designation for aquatic toxicity and degradation studies for component E lead to the score “moderate” for persistence.

Measured BCF values for the components C and D do not exceed 364. The US EPA states that the bioaccumulation score “high” is based on a QSAR-estimated BAF of 18,000 for component E (usually values > 5000 trigger “very high”), but states also that the “estimated low BCF value [presumably for component E] is consistent with the limited water solubility estimates”. The Log Kow for component E has been estimated at 11, thus being greater than the methodology cut-off value of 10, and measured Log Kow values are not available. Being conservative, we assign the score “very high” based on the estimated BAF.

Overall hazard scoring
An overall hazard score = 1 has been assigned because the substance meets criterion e) for Benchmark 1 by scoring "high" for T (Group I Human).

4.7.4 Fyrol™ HF-5

Technical description

CAS No	Confidential
EC No	-
Chemical name	Proprietary Phosphorus Ester Blend
Structural formula	-
General formula	-
Phosphorous content	14% (Fyrol™ HF-5)
Abbreviation, synonyms	
FR products and manufacturers	Fyrol™ HF-5 (ICL-IP Europe)
Registered tonnage, t/year	-
Pinfa Product Selector	Not available
Other information on substrate	Flexible polyurethane foam. Its high molecular weight and low fogging potential is advantageous in demanding flexible foam applications where low VOC emissions are required.
End applications	Furniture, automotive
Reactive/additive	Additive
Health env. profiles	Flame retardants used in flexible polyurethane foam (US EPA, 2015)
Availability	-
Flame retardancy	It is highly effective in producing flame retardant flexible polyurethane foam meeting both Cal TB 117 and MVSS-302 criteria. (ICL-IP Europe)
Halogen-containing flame retardants for the same application (examples)	TCPP, TDCP

Hazard profile

The screening of Fyrol™ HF-5* by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 36
SCORINGOF FYROL™ HF-5* USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	M	L	M	H	L	DG	M	DG	M	L	DG	L	M	VH	VH	VH	M	1

C = Carcinogenicity	ST = Systemic toxicity	AA = Acute aquatic toxicity
M = Mutagenicity	N = Neurotoxicity	CA = Chronic aquatic toxicity
R = Reproductive toxicity	SnS = Skin sensitization	P = Persistence
D = Developmental toxicity	SnR = Respiratory sensitization	B = Bioaccumulation
E = Endocrine activity	IrS = Skin irritation	
AT = Acute mammalian toxicity	IrE = Eye irritation	

Comments to hazard profile scores
The flame retardant Fyrol™ HF-5* contains 2 confidential components (Confidential A, Confidential B), both with confidential CAS No. Experimental and measured data for the single compounds are listed in the US EPA report (2015), but are summarized in one hazard table here. The substance is a mixture that contains polymeric components, and both residual monomers, unreacted starting material and low MW oligomers are expected to be present in the product.

No experimental data were available for the endpoint carcinogenicity. However, Confidential B is estimated to have uncertain potential for carcinogenicity based on analogy to related chemicals and professional judgement, while confidential A is estimated to have low potential for carcinogenicity.

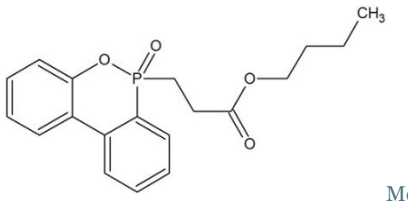
For all other human endpoints, experimental data are available for either one or even both components. In addition to experimental data for component B, a metabolite of the test substance is listed as a suspected endocrine disruptor by the EU. The potential for endocrine activity for Confidential A is uncertain. In accordance with the GreenScreen profiles of 4.1.3 Poly(m-phenylene methylphosphonate), CAS No. 63747-58-0), and 4.2.6 Resorcinol bis-diphenyl phosphate, CAS No. 57583-54-7), we have assigned the score "high" to endocrine activity, based on the metabolite.

The evaluation of aquatic toxicity is based on experimental data. The persistence designation is based on experimental data with the higher MW components (MW >1,000). No experimental data are available on bioaccumulation, a QSAR-estimated fish BCF of 1,300 for the n=1 oligomer leads to the "moderate" score for bioaccumulation.

Overall hazard scoring
An overall hazard score = 1 has been assigned because the substance fulfils criterion c) "very high" for both P and T, as well as criterion e) "high" T (Group I Human).

4.7.5 6H-Dibenz[c,e][1,2]oxa-phosphotin-6-propanoic acid, butyl ester, 6-oxide, CAS No. 848820-98-4

Technical description

CAS No	848820-98-4
EC No	805-659-5
Chemical name	6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide
Structural formula	 Metadynea
General formula	C19H21O4P
Phosphorous content	Min. 8.5
Abbreviation, synonyms	DOB11
FR products and manufacturers	DOPO-AC4, DOB11, Metadynea Austria GmbH Levagard TP LXS 51114, Lanxess
Registered tonnage, t/year	10 – 100
Pinfa Product Selector	Not included in PPS
Other information on substrate	Polyesters, PUR and epoxy-systems
End applications	DOB11 is especially suited for polyesters, PUR and epoxy-systems intermediate (Metadynea, 2014a).
Reactive/additive	Additive
Health env. profiles	Screened as part of this study (see below)
Availability	Available from several manufacturers Product introduction into the flexible PUR market has just started; only lab experience is available (Lassen et al., 2015).
Flame retardancy	Gas phase inhibitor. Loading approx. twice the concentration of TDCP to pass the automotive MVSS 302 test (Lassen et al., 2015)
Halogen-containing flame retardants for the same application (examples)	TCPP, TDCP DecaBDE, DBDPE, EBTEBPI (all in combination with antimony trioxide) and others

Hazard profile

The screening of this alternative by the modified GreenScreen® methodology was based on information compiled according to the information sources described in 3.2.1. The full data set from the data collection including justification of the scoring is enclosed as Appendix 9 to this report.

TABLE 37
SCORING OF 6H-DIBENZ[C,E][1,2]OXAPHOSPHORIN-6-PROPANOIC ACID, BUTYL ESTER, 6-OXIDE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
DG	DG	DG	DG	DG	**L**	DG	DG	DG	DG	**L**	DG	**H**	DG	**M**	**M**	**H**	**L**	2

Comments to hazard profile scores
A notified classification is available for 6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide: Skin Irrit. 2 (H315; 29 notifiers), Aquatic Chronic 3 (H412; 28 notifiers).

Only very limited data are available for the substance. Experimental data lead to the scores of Group II Human, ecotoxicity and fate. Some of the endpoint scores are supported by QSAR estimates.

Overall hazard scoring
A Benchmark score = 2 has been assigned because the substance does not fulfil any criteria behind Benchmark 1, but meets criterion c) of Benchmark 2 by scoring " high" for persistence, "high" for an endpoint in Group II Human and "moderate" for ecotoxicity (only "moderate" toxicity scores are required for criterion c) of Benchmark 2).

4.8 Halogenated flame retardants

4.8.1 Decabrominated diphenyl ether (decaBDE), CAS No. 1163-19-5

Hazard profile

The screening of decaBDE by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for the flame retardant decabromodiphenyl ether (DecaBDE; US EPA, 2014b).

TABLE 38
SCORING OF DECABDE USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	**L**	**L**	**H**	**H**	**L**	DG	**M**	DG	L	**L**	DG	**L**	**L**	L	L	**VH**	H	1

Comments to hazard profile scores

All endpoint scores, except neurotoxicity, aquatic toxicity and bioaccumulation are based on experimental data presented in the report (US EPA, 2014b).

With respect to endocrine activity, DecaBDE is listed as a Category 2 (Evidence of potential to cause endocrine disruption) on the EU priority list of substances. Moreover, some metabolites of decaBDE are known to produce estrogenic effects (US EPA, 2014b). We therefore assign the score “high” to this endpoint.

Given the low water solubility of the substance, no aquatic effects at saturation are expected (US EPA, 2014b).

Overall hazard scoring

An overall hazard score = 1 has been assigned because the substance meets criterion c) and e) for Benchmark 1 by scoring "high" for developmental toxicity (Group I Human) and “very high” for persistence.

4.8.2 Tetrabromobisphenol A (TBBPA), CAS No. 79-94-7

Hazard profile

The screening of TBBPA by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for halogenated flame retardant in printed circuit boards (US EPA, 2014c).

TABLE 39
SCORING OF TBBPA USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	L	M	H	L	DG	L	L	L	L	DG	L	M	VH	H	H	M	1

Comments to hazard profile scores

All scores are based on experimental data. The scores of fate endpoints are further supported by estimated data.

The US EPA did not assign a score on endocrine activity, but listed > 20 studies relating to this endpoint. Both whole animal and *in vitro* studies indicate that TBBPA may exhibit endocrine activity.

Overall hazard scoring

An overall hazard score = 1 has been assigned because the substance meets criterion e) for Benchmark 1 by scoring "high" for T (Group I Human).

4.8.3 Hexabromocyclododecane (HBCDD), CAS No. 25637-99-4 and 3194-55-6

Hazard profile

The screening of HBCDD by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for hexabromocyclododecane (HBCDD) (US EPA, 2014c).

TABLE 40
SCORING OF HBCDD USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	M	H	H	L	DG	M	M	M	L	DG	L	L	VH	VH	H	VH	1

Comments to hazard profile scores

There are 16 possible hexabromocyclododecane (HBCDD) isomers. CAS No. 25637-99-4 is assigned to a non-specific mixture of all HBCDD isomers and CASRN 3194-55-6 is assigned to the mixture of 1,2,5,6,9,10-HBCDD isomers. The US EPA report accounts for differences in the fate and behaviour in the environment, and the potential for toxic effects for individual HBCD isomers.

The carcinogenicity score is derived from an estimation and an insufficient, but indicative mouse study. The score for neurotoxicity is based on structural alert and professional judgment. For all other human health endpoints, sufficient experimental data have been available in the US EPA report. *In vitro* and *in vivo* studies demonstrated endocrine activity, thus we mark this endpoint with "High". Experimental data give rise to the environmental scores.

Overall hazard scoring

An overall hazard score = 1 has been assigned because the substance fulfils the criteria a), d) and e) by scoring “very high” for aquatic toxicity and bioaccumulation and “high” for toxicity (Group I Human).

4.8.4 Tris (1-chloro-2-propyl) phosphate (TCCP), CAS No. 13674-84-5

Hazard profile

The screening of TCCP by the modified GreenScreen® methodology was made using the data for the substance collected and presented by US EPA in its assessment of alternatives for flame retardants used in flexible polyurethane foam (US EPA, 2015).

TABLE 41
SCORING OF TCCP USING THE PROPOSED MODIFIED METHODOLOGY

Group I Human					Group II and II* Human									Ecotox		Fate		Overall Hazard Score
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	
						single	repeat*	single	repeat*									
M	L	H	H	M	L	DG	M	M	M	L	DG	L	L	M	M	H	L	1

Comments to hazard profile scores

There were no experimental data located for carcinogenicity; carcinogenic effects cannot be ruled out. The US EPA therefore applies the score "moderate" to this endpoint. The neurotoxicity scores are based on experimental data and supported by weight of evidence from structural alert for organophosphates. Endocrine activity was demonstrated in several cell assays.

Measured and estimated BCF and BAF values are < 100, corresponding to the "very low" bioaccumulation designation (the US EPA assigns "low" according to their bioaccumulation criterion). However, the authors also state that the designation is not consistent with results of biomonitoring studies, since TCCP has been detected in herring gull eggs and human breast milk (US EPA, 2015). Considering the measured log Kow (2.68, 2.59 and 3.33), we maintain the "low" hazard designation.

Overall hazard scoring

An overall hazard score = 1 has been assigned because the substance meets criterion e) by scoring "high" for T (Group I Human).

5. Phosphorous flame retardants and smoke by fire

5.1 Formation of particles and hazardous gases by fire

Most fire deaths are caused by inhalation of smoke. Often smoke incapacitates so quickly that people are overcome and cannot make it to an otherwise accessible exit. Synthetic materials being commonplace in buildings, construction and means of transport form especially dangerous smoke. As a fire grows it will often consume most of the available oxygen, slowing the burning process, and this "incomplete combustion" leads to the formation of toxic gases.

Smoke is made of components that can each be lethal in its own way (NFPA, 2015):

- **Particles**: Unburned, partially burned, and completely burned substances can be so small they penetrate the respiratory system's protective filters, and lodge in the lungs. Some are actively toxic; others are irritating to the eyes and digestive system.
- **Vapours**: Foglike droplets of liquid can poison if inhaled or absorbed through the skin.
- **Toxic gases:** The most common, carbon monoxide (CO), can be deadly, even in small quantities, as it replaced oxygen in the bloodstream. Hydrogen cyanide results from the burning of plastics, such as PVC pipe, and interferes with cellular respiration. Phosgene is formed when household products, such as vinyl materials, are burned. At low levels, phosgene can cause itchy eyes and a sore throat; at higher levels it can cause pulmonary oedema and death.

Key toxic products in fires, as summarised by Purser (2009), are:

- Products threatening survival during and immediately after a fire:
  - **Asphyxiant gases**: CO, HCN, CO_2 , low oxygen
  - **Irritants**:
    - acid gases – HCl, HBr, HF, COF_2 , H_3PO_4, SO_2 , NOx
    - organic irritants - acrolein, formaldehyde, crotonaldehyde, phenol, styrene
  - **Particulates** (especially ultrafine particles)
- Products causing environmental contamination, with long term health implications for repeated exposure during firefighting or post-fire investigation
  - Benzene, isocyanates, PCBs, PAHs, dioxins and furans, aldehydes
  - Inhalable fibres: asbestos, ceramic, mineral, carbon fibre
  - Particulates, metals

The possible effects of the toxicants are different for the different fire zones as summarised by Purser (2009):

- **Zone 1**: Inside fire compartment. Exposure to effluent fire plume lethal within minutes (due to asphyxiant and irritant gases).
- **Zone 2**: Outside immediate fire compartment or building. Exposure to effluent plume with dilution factor of 50-100 times that inside fire (hazard from brief exposure to more concentrated "downwashed" smoke plumes) canteen.
- **Zone 3**: Surrounding area of city exposed to downwind plume) – Potential minor health hazards to large exposed population from much more diluted plume

Asphyxiant gases (carbon monoxide and hydrogen cyanide) are the main Zone 1 killers, but are relatively harmless at the 50-100 dilution levels in the smoke plume outside the immediate fire zone. Irritant gases and associated particulates are also lethal at Zone 1 concentrations, but still present significant health hazards at Zone 2 (and to some extent at Zone 3 concentrations). Irritant gases cause inflammation of eyes and respiratory tract (potential acute and chronic bronchitis, chronic obstructive lung diseases, such as fibrosis or emphysema, RADs (reactive airway disfunction syndrome). Other exposures toxic at Zone 2 concentrations or during post-fire investigation are (Purser, 2009):

- Sensitizers including formaldehyde and isocyanates leading to asthma
- Organic carcinogens: PAHs, dioxins, dibenzofurans, metals
- Ceramic and asbestos fibres: lung fibrosis, pleural cancers
- Ultrafine particulates and CO: risk of angina and heart attacks

5.1.1 Flame retardant mechanism of phosphorous flame retardants

As described by Clariant Produkte (2015), flame retardants may slow down or even interrupt the combustion process by physical or chemical action in the solid, liquid or gas phase. They interfere during heating, decomposition, ignition or flame spread with the course of the fire. The most important processes are:

- **Physical action** by **cooling** (endothermic process of FR decomposition) or **dilution** of the substrate in the gas phase (i.e. formation of water) and the solid phase (alumina trihydrate and magnesium hydroxide), or by **coating** the substrate (shielding it against the attack of oxygen and heat) with phosphorous and nitrogen compounds.
- **Chemical action** in the gas phase interferes with the combustion processes by eliminating the high energy H and OH radicals by halogen halides from halogenated flame retardants, metal halogen compounds from antimony trioxide, and phosphorous-containing fragments from phosphorous flame retardants ("flame poisoning"). In the solid phase, the flame retardant forms a carbonaceous layer on the surface of the polymer by dehydration, formation of double bonds, thus initiating cyclization and cross-linking (phosphorous, nitrogen compounds, intumescent systems.

The benefit of fire retardant treatments is mainly to reduce the probability that a heat or ignition source will initiate a growing spreading fire (Purser, 2009). If the initial ignition resistance is overcome the presence of flame retardants may reduce the rate of fire growth. For some flame retardants mechanism in this phase the presence of flame retardants may also slow the burning process leading to the increased formation of toxic gases. With respect to toxic product yields the ideal fire retardant system according to Purser (2009) acts in the solid phase and minimises the release of organic fuel vapours and acid gases. Systems that lead to reduced organic emissions relative to the parent polymer include inert fillers, alumina trihydrate systems, char forming or layer forming systems locking up fuel carbon such as borax/boric acid and char forming nitrogen-phosphorus systems, and nano-clay systems (Purser, 2009).

Phosphorous-containing flame retardants are active mainly in the solid phase of the polymer and influence pyrolysis and char formation (Troitzsch, 2004). In the solid phase they form phosphoric and related acids by thermal degradation, and water is released from the substrate in the solid phase, which act as a "heat sink". They form a thin glassy coating, which is a barrier that lowers the evolution of combustible gases in the gas phase and limits the diffusion of oxygen and the heat transfer (Troitzsch, 2004). Specific phosphorus flame retardants such as the metal phosphinates may also act in the gas phase by the formation of P and PO radicals interrupting the radical chain mechanism of the combustion process (Clariant Produkte, 2014). Vapour phase flame inhibition is enhanced by the presence of nitrogen and halogens (Purser, 2014).

The mechanism of intumescent flame retardant systems which are typically a combination of phosphorus and nitrogen compounds is to form a isolating carbon layer which reduce smoke formation (Pinfa, 2011). In the event of fire the flame retardants react together as a result of the temperature increase to form a carbon foam. This foam attains a thickness of 10 to 100 times of the originally applied coating and insulates the substrate material through its low thermal conductivity. Intumescent coating systems are often used to protect steel from overheating, but can also be applied to timber surfaces, thereby acting as an FR coating, inhibiting ignition, surface spread of flame, and heat propagation. These coatings consist of a carbon supplier (starch, polyol, or pentaerythritol), ammonium polyphosphate, and melamine as an expanding agent (Turner, 2014).

5.2 The influence of phosphorous flame retardants on the formation of smoke and toxic gases

Depending upon the flame retardant system, as mentioned above, the phosphorous flame retardants acts partly in the solid phase by formation of a char and partly in the vapour phase. The influence of the phosphorous flame retardants on the formation of the toxic gases and other smoke components depends on the specific systems. A summary of fire performance of phosphorous flame retardants is shown in Table 42. Whereas non-halogenated phosphorous flame retardants in general reduce the yields of toxic combustion products compared to materials without flame retardants, phosphorous halogenated flame retardants increase the yields.

TABLE 42
SUMMARY OF FIRE PERFORMANCE OF PHOSPHOROUS FLAME RETARDANTS (BASED ON TURNER, 2014)

	Reduces fire probability	Reduces fire size	Yields of toxic combustion products	Yields of environmental toxic products
Phosphorous and phosphorous/nitrogen FRs	Yes	Yes, by char formation and in gas phase	Some reduced	Reduced
Phosphorous halogen	Yes	Yes, mainly gas phase	Increased	Increased
Ammonium polyphosphate	Yes	Yes, with char formation	Reduced	Reduced
Intumescent coatings	Yes	Yes	No	None

Char formation

The main feature of phosphorous flame retardants is char-forming activity, sometimes combined with foaming-up (intumescence), which then forms a protective top layer on the plastic surface. The advantage of such a solid-phase mechanism is that it causes less release of smoke and off-gases in a developing fire situation, thus keeping secondary fire damage as low as possible (Schmitt, 2007).

The main advantages of intumescent phosphor-based flame retardants in polyolefins (polyethylenes and polypropylenes) are as summarised by Schmitt (2007):

- Very low smoke density in the developing phase of a fire
- No corrosivity of the smoke/off gases, which is important for electronics
- Low heat-release rates, therefore reduced speed of fire spread.

The flame performance of phosphorous flame retardants as compared with halogenated flame retardants have been studied in several studies.

Molyneux et al. (2014 a,b) burned standard industry formulations of flame retarded aliphatic polyamides, meeting UL 94 V-0 under controlled conditions, and the yields of the major asphyxiants, carbon monoxide (CO) and hydrogen cyanide (HCN) was quantified. The study showed that in

aliphatic polyamides, brominated flame retardants with an antimony oxide synergist, which interfere with gas-phase free radical reactions, produce high yields of both carbon monoxide and hydrogen cyanide. In contrast, the aluminium phosphinate/melamine polyphosphate combination, which is believed to act in both gas and condensed phases, caused a significantly smaller increase in the yields of these two main asphyxiants. According to the authors it is crucial, in the context of the flame inhibition that the phosphorus system reduces the H and O radical concentrations without a corresponding decrease in the OH radical concentration. Moreover, while the phosphorus flame retardant is effective as an ignition suppressant at lower temperatures (corresponding to early flaming), this effect "switches off" at high temperatures, minimising the potential increase in fire toxicity, once the fire develops. The work furthermore showed that hydrogen cyanide (HCN) was the major contributor to the toxicity for all fire retarded PA materials reported in the study, even in well-ventilated conditions, although the contribution from CO from materials flame retarded with brominated flame retardants was also significant. By estimating the overall fire toxicity (using toxicity equivalency factors for the different toxic compounds), the study showed that the polyamide with the flame retardant containing bromine and antimony caused a significant increase in the fire toxicity, compared to the material flame retarded by the aluminium phosphinate/melamine polyphosphate blend. (Molyneux et al., 2014 a).

With the aims to develop halogen-free poly(1,4-butylene terephthalate) (PBT) composites with enhanced flame retardancy Yang et al. (2011) produced flame retarded PBT using aluminium hypophosphite (AHP) and melamine derivatives (melamine polyphosphate and melamine cyanurate). A loading of 20 wt % flame retardant mixture fulfilled the PBT composites high limited oxygen index (LOI) and V-0 classification in UL 94 testing. For the PBT composites with the incorporation of aluminium hypophosphite (AHP) and melamine derivatives, the heat release capacity (HRC), which is an indicator of a material fire hazard, was significantly reduced, and the intensities of a variety of combustible or toxic gases detected by TG-IR technique were remarkably decreased. (Yang et al., 2011)

Even the yield of smoke is lower when using phosphorous flame retardants as compared to halogenated flame retardants in some systems the addition of the flame retardants result in higher smoke formation than in the non-flame retarded system. Polyamide 6 (PA 6) and polypropylene (PP) containing fire retardants, nanofillers or a combination of both additives were tested under three different fire conditions, to determine the effect of additives on the soot production or toxic product yields. In all ventilation conditions the virgin polymer produces the least amount of soot, both the additives used (fire retardant and nanoclay) increase the amount of soot, mainly within 0.5–1.0 μm range, for each fire condition. (Rhodes et al. 2011).

An important consideration is the form in which the vapour phase phosphorus is released during fires. This has according to Purser (2014) been little studied, but in general phosphorus and organic phosphorous compounds are readily oxidized, so that the main product is P_2O_5, which then hydrolyses to H_3PO_4. This is moderately toxic, and may make some small contribution to overall toxicity of fire effluents from treated materials. Phosphine (PH_3) is another toxic compound detected in some fire effluents (a highly toxic substance causing lung oedema. Some traces of organophosphorus compounds have been detected in the combustion products from burning materials, but toxicity test protocols designed to detect neurotoxic compounds have not been used with combustion atmospheres. One serious exception is the finding that any phosphorus source when combined with a trimethylol polyol can produce a potent neurotoxic class of bicyclophosphate esters in combustion products. In practice this has been a potential problem only with certain turbine lubricants containing trimethylol (Purser, 2014)

Low smoke, zero halogen cables have been growing strongly in Europe. According to EFRA (2015) bis-aryl phosphates (BDP, CDP) provide good low temperature flexibility in thermoplastic elastomers and rubbers such as EPDM, SBR, NBR or TPU, and are also recommended for low smoke

formulations. (EFRA, 2015). Even the phosphorous flame retardants result in lower smoke yield, mainly non-phosphorous inorganic flame retardants are used as smoke suppressants in flame retardants formulations. For wires and cables made of polyolefins like LDPE, LLDPE or PP, mineral flame retardants are often used – mainly finely precipitated aluminium tri-hydroxide (ATH) and magnesium dihydroxide (MDH). While relatively inexpensive, they usually require high loadings of up to 60% of the weight of the final material. Zinc borate can be used in combination with ATH and MDH to enhance smoke suppression (EFRA, 2015).

Abbreviations and acronyms

ABS	Acrylonitrile-butadiene-styrene
ACToR	Aggregated Computational Toxicology Resource
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ASTDR	Agency for Toxic Substance & Disease Registry
AHP	Aluminum hypophosphite
ATH	Aluminium trihydrate
ATO	Antimony trioxide, Sb2O3
APP	Ammonium polyphosphate
BAF	Bioaccumulation factor
BAPP	Bisphenol A bis(diphenyl phosphate)
BCF	Bioconcentration factor
BPA-BDPP	Bisphenol A bis(diphenyl phosphate)
BPBP	Phosphoric acid, mixed esters with [1,1'-bisphenyl-4,4'-diol] and phenol
BM	Benchmark
C&L	Classification and labelling
CAS	Chemical Abstracts Service
CB	Circuit boards
CDP	Cresyl diphenyl phosphate
CHIRP	Chemical Risk Information Platform
CICAD	Concise International Chemical Assessment Documents
CLP	Classification, labelling and packaging
CMR	Carcinogenic, mutagenic and reprotoxic
CO	Carbon monoxide
CO2	Carbon dioxide
DBDPE	Decabromodiphenyl ethane
DBDPE	Ethane-1,2-bis(pentabromophenyl)
Deca-BDE	Decabromodiphenyl ether
DfE	Design for the Environment [progamme]
DG	Data gap
DOT	US Department of Transportation Hazardous Materials Regulations
EBTEBPI	Ethylene bis(tetrabromophthalimide)
ECHA	European Chemicals Agency
ED	Endocrine disruption
EDAP	Ethylenediamine, salt with phosphoric acid
EEE	Electrical and electronic equipment
EFRA	European Flame Retardants Association
EHC	Environmental Health Criteria
EPA	Environmental Protection Agency
EPDM	Ethylene propylene diene monomer (M-class) rubber
EPI	Estimation Programs Interface
EPS	Expanded polystyrene
EVA	Ethylene-vinyl acetate
FDA - ED	US Food and Drug Administration - Endocrine Disruptor Knowledge Base
FR	Flame retarded or flame retardants
GHS	Global Harmonized System
HBCDD	Hexabromocyclododecane (same as HBCD)
HCL	Hydrochloric acid

HF	Hydrogen fluoride
HIPS	High impact polystyrene
HIPS/PPO	Copolymer of HIPS and PPO
HSDB	Hazardous Substances Data Bank
IARC	International Agency for Research on Cancer
INCHEM	Chemical Safety Information from Intergovernmental Organizations
IRIS	Integrated Risk Information System
JECFA	Joint Expert Committee on Food Additives
LC50	Lethal concentration which causes the death of 50% of a group of test animals
LOUS	List of Undesirable Substances
MAK	Maximum permissible concentration of a substance as a gas, vapour or aerosol in the air at the workplace (derived from German)
MDH	Magnesium dihydroxide
MW	Molecular weight
NGO	Non-governmental organisation
NIOSH	National Institute for Occupational Safety and Health
OECD	Organisation for Economic Co-operation and Development
PAH	Polyaromatic hydrocarbons
PAN	Pesticide Action Network Pesticide Database
PBT	Persistent, bioaccumulative and toxic
PBT	Polybutylene terephthalate
PC	Polycarbonate
PC/ABS	Copolymer of PC and ABS
PCB	Polychlorinated biphenyls
PE	Polyethylene
PDM	Poly
PET	Poly(ethylene terephthalate)
Pinfa	Phosphorus, Inorganic and Nitrogen Flame Retardants Association
PP	Polypropylene
PPO	Polyphenylene oxide
PPS	Pinfa Product Selector
PS	Polystyrene
PUR	Polyurethane
PVC	Polyvinyl chloride
QSAR	Quantitative structure–activity relationship
RDP	Resorcinol bis(diphenylphosphate)
REACH	Registration, Evaluation, Authorisation and Restriction .of Chemicals
SIDS	Screening Information Data Set
Stot	Specific target organ toxicity
SVHC	Substances of very high concern
TBBPA	Tetrabromobisphenol A
TBPP	Tris (p-t-butylphenyl) phosphate
TCP	Tricresyl phosphate
TCPP	Tris(2-chloro-1-methylethyl) phosphate
TDCP	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate
TMPP	Tricresyl phosphate
ToxRefDB	US EPA Toxicity Reference Database
TPU	Thermoplastic polyurethane
UKPID	UK Poison Information Documents
UL 94	Underwriters Laboratories 94 standard
US EPA	United States Environmental Protection Agency
USA	United States of America
vPvB	Very persistent and very bioaccumulative
XPS	Extruded polystyrene

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Appendix 1 Summary hazard profiles from US EPA

The screening level hazard summary for flame retardants used in PUR foams as alternatives to penta-BDE prepared by the US EPA (2015) are shown in the following table. The table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation by-products. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table.

TABLE 43
SCREENING LEVEL HAZARD SUMMARY FOR SELECTED HALOGENATED AND NON-HALOGENATED PHOSPHOROUS FLAME RETARDANTS USED IN PUR FOAMS AS ALTERNATIVES TO PENTA-BDE (US EPA, 2015) *1

Chemical	CAS No	Human Health Effects											Aquatic Toxicity		Environ-mental Fate	
		Acute toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Phosphorus flame retardants																
Ammonium polyphosphate (APP) ¥	68333-79-9	L	L	L	L	L	L	L[d]	L		VL	L	L	L	VH	L
Triphenyl phosphate (TPP) †	115-86-6	L	M	L	L	L	L	H	L		L	VL	VH	VH	L	M
Tricresyl phosphate (TCP) 1	1330-78-5	M	L	L	H	M	M	H	M		L	L	VH	VH	M	H
Isopropylated triphenyl phosphate (IPTPP) †	68937-41-7	L	M	L	H	H	H	H	L		L	L	VH	VH	M	H
Tris (p-t-butylphenyl) phosphate (TBPP)	78-33-1	L	M	L	M	L	M	H	M		L	M	VH	VH	M	H
Diethyl bis(2hydroxyethyl) ami-nomethylphosphonate	2781-11-5	L	M	M	L	L	M	M	M		L	VL	L	L	H	L
Oligomeric ethyl ethylene phosphate	184538-58-7	L	L	M	L	M	M	L[d]	L		M	L	L	L	VH	L
Oligomeric phosphonate polyol	363626-50-0	L	M	M	L	M	M	L	L		L	VL	L	L	M	L
New-to-Market Proprietary Mixtures																
Emerald Innovation™ NH-1	Proprietary	H	M	L	M	L	M	H	M		M	M	VH	VH	M	H
Confidential C	Confidential	H	M	L	M	VL	M	L	M		M	M	H	H	L	L
Confidential D	Confidential	L	M	L	L	L	L	H	L		L	VL	VH	VH	L	M
Confidential E	Confidential	L	M	L	L	L	M	M	M		VL	M	VH	VH	M	H
Fyrol™ HF-5	Proprietary	L	M§	M	L	M	M§	M[d]	L		M	L	VH	VH	VH	H‡
Confidential A	Confidential	L	L	M	L	L	M	L	L		M	L	L	L	VH	L
Confidential B	Confidential	L	M	L	L	M	M	M	L		L	VL	VH	VH	M	H
Halogenated Flame Retardants - Firemaster® 550 Components																

Firemaster® 550*	Mixture	L	M	M	H	H	H	H	M		L	L	VH	VH	H	H
Benzoic acid, 2,3,4,5-tetrabromo-, 2-ethylhexyl ester (TBB) ¥	183658-27-7	L	M	L	M	M	M	M	M		L	L	L	L	H	H
Di(2-ethylhexyl) tetrabromophthalate (TBPH) ^ ¥	26040-51-7	L	M	M	M	M	M	M	L		L	L	L	L	H	H
Isopropylated triphenyl phosphate (IPTPP) ^	68937-41-7	L	M	L	H	H	H	H	L		L	L	VH	VH	M	H
Triphenyl phosphate (TPP) ^	115-86-6	L	M	L	L	L	L	H	L		L	VL	VH	VH	L	M
Halogenated Flame Retardants - Chlorinated Phosphorus Alternatives																
Tris (2-chloroethyl) phosphate (TCEP)	115-96-8	H	H	M	M	H	M	M	L		L	L	H	H	M	L
Tris (2-chloro-1-methylethyl) phosphate (TCPP)	13674-84-5; 6145-73-9	L	M	L	H	H	M	M	L		L	L	M	H	H	L
Tris (1,3-dichloro-2-propyl) phosphate (TDCPP)	13674-87-8	L	H	M	H	M	L	H	L		L	L	H	H	H	L
Phosphoric acid, P,P'-[2,2-bis(chloromethyl)-1,3propanediyl] P,P,P',P'-tetrakis(2-chloroethyl) ester (V6)	38051-10-4	L	M	L	M	H	L	M	L		L	L	M	H	H	L

Notes from the cited report:
VL = Very Low hazard **L** = Low hazard **M** = Moderate hazard **H** = High hazard **VH** = Very High hazard –
Endpoints in coloured text (**VL, L, M H**, and **VH**) were assigned based on empirical data.
Endpoints in black (VL, L, M, H, and VH) were assigned using values from predictive models and/or professional judgement.

* This mixture is made up of four components contained in the hazard summary table. Hazard designations in bold and colour are based on test data for the mixture, as summarized in the hazard profiles for the components. Hazard designations in italics are based on the most conservative results from one of the four components.

^ This component of Firemaster® 550 may be used alone or in other mixtures as an alternative.

¥ Aquatic toxicity: EPA/DfE criteria are based in large part upon water column exposures, which may not be adequate for poorly soluble substances such as many flame retardants that may partition to sediment and particulates.

1 This assessment also includes information for other methylated triphenyl phosphate isomers (phosphoric acid, bis(methylphenyl) phenyl ester (CASRN 26446-73-1) and phosphoric acid, methylphenyl diphenyl ester (CASRN 26444-49-5))

TABLE 44
SCREENING LEVEL HAZARD SUMMARY FOR decaBDE AND BROMINATED FLAME RETARDANT ALTERNATIVES (US EPA, 2014A) *1
THIS TABLE ONLY CONTAINS INFORMATION REGARDING THE INHERENT HAZARDS OF FLAME RETARDANT CHEMICALS. THE CAVEATS LISTED IN THE LEGEND AND FOOTNOTE SECTIONS MUST BE TAKEN INTO ACCOUNT WHEN INTERPRETING THE HAZARD INFORMATION IN THE TABLE.

Chemical	CAS No	Human Health Effects											Aquatic Toxicity		Environ-mental Fate	
		Acute toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
DecaBDE and discrete BFR alternatives																
Decabromodiphenyl ether, decaBDE	1163-19-5	L	M	L	L	H	H	M	L		L	L	L	L	VH	H
Bis(hexachlorocyclopentadieno) cyclooctane,	13560-89-9	L	M§	M§	VL	VL	L	M	L		VL	L	L	L	VH	H
Decabromodiphenyl ethane, DBDPE	84852-53-9	L	M§	L	L	VL	H§	L	L		VL	VL	L	L	VH	H
Ethylene (bistetrabromophthalimide), EBTEBPI	32588-76-4	L	M§	L	L	L	M§	L	L		VL	VL	L	L	VH	H
Tetrabromobisphenol A bis (2,3-dibromopropyl) ether, TBBPA-BDBPE	21850-44-2	L	M	M	M	M	L	M	M		L	L	L	L	VH	H
Tris(tribromoneopentyl) phosphate, TTBNPP	19186-97-1	L	M	M	L	H	H	M	H		L	L	L	L	H	M
Tris(tribromophenoxy) triazine, TTBP-TAZ	25713-60-4	L	L	L	L	L	L	L	L		L	VL	L	L	VH	H
Polymeric BFRs																
Brominated epoxy resin end-capped with tribromophenol	135229-48-0	H	L	L	L	L	L	Md	L		L	VL	L	L	VH	L
Brominated polyacrylate	59447-57-3	L	L	L	L	L	L	Md	L		L	L	L	L	VH	L
Brominated polystyrene	88497-56-7	L	L	L	L	L	L	Md	L		L	L	L	L	VH	L
Confidential brominated epoxy polymer #1	Confidential	L	L	L	L	L	L	Md	L		L	L	L	L	VH	L
Confidential brominated epoxy polymer #2	Confidential	L	L♦	L♦	L♦	L♦	L	M♦d	L♦	♦	L	L	L♦	L♦	VH	L♦
Confidential brominated epoxy polymer Mixture	Confidential	L	L♦	L♦	L♦	L♦	L	M♦d	L♦	♦	L	L	L♦	L♦	VH	L♦

Chemical	CAS No	Human Health Effects											Aquatic Toxicity		Environ-mental Fate	
		Acute toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Confidential brominated epoxy polymer Mixture	Confidential	L	L♦	L♦	L♦	L♦	L	M♦d	L♦	♦	L	L	L♦	L♦	VH	L♦
Confidential brominated polymer	Confidential	L	L¤	L	L¤	L¤	L¤	L¤	L	L	L	VL	L	MT¤	VHT	MT¤
TBBPA glycidyl ether, TBBPA polymer	68928-70-1	L	L♦	L♦	L♦	L♦	L	M♦d	L	♦	L	L	L♦	L♦	VH	L♦
Organic phosphorus or nitrogen flame retardants (PFRs or NFRs) alternatives																
Substituted amine phosphate mixture	Confidential	H	M	M	M	M	L	M	M	M§	M§	VH	M	L	H	L
Triphenyl phosphate	115-86-6	L	M	L	L	L	L	M	L		L	VL	VH	VH	L	M
Bisphenol A bis-(diphenyl phosphate), BAPP	181028-79-5	L	L	L	L	L§	L	L	L		L	L	L	L	H	HO
Melamine cyanurate	37640-57-6	L	M	M	M§	M§	L	H	L		L	L	L	L	VH	L
Melamine polyphosphate	15541-60-3	L	M	M	L§	L	L§	M	L		L	VL	L	L	H	L
N-alkoxy hindered amine reaction products	191680-81-6	L	M	L	H	H	L	H	L		L	VL	H	H	H	H†
Phosphonate oligomer	68664-06-2	L	M	L§	L¥	L¥	M†	L*§	L*§		M§†	M†	L¥	H†	VH	H†
Polyphosphonate	68664-06-2	L	¤	L	L	L	L	Md	L		L	L	L	L	VH	L
Poly[phosphonate-co-carbonate]	77226-90-5	L	L	L	L	L	L	Md	L		L	L	L	L	VH	L
Resorcinol bis-diphenylphosphate	125997-21-9	L	M§	L	L	VL	M§	M	L		L	VL	VH	H†	M	H†
Inorganic flame retardant alternatives																
Aluminium diethylphosphinate	225789-38-8	L	L	L	L	M	M	L	L		L	VL	M	M	HR	L
Aluminium hydroxide	21645-51-2	L	L	L	L	L	M	L	L		VL	VL	M	M	HR	L
Ammonium polyphosphate	68333-79-9	L	L	L	L	L	L	Md	L		VL	L	L	L	VH	L
Antimony trioxide1	1309-64-4	L	L*	L	L	L	L	M	L		L	M	M	M	HR	L

Chemical	CAS No	Human Health Effects											Aquatic Toxicity		Environ-mental Fate	
		Acute toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Magnesium hydroxide	1309-42-8	L	L	L	*L*	*L*	*L*	L	*L*		M	*M*	*L*	*L*	*H*[R]	*L*
Red phosphorus	7723-14-0	VH	*L*	*M*	*L*	*L*	*L*	L	L		M	H	L	L	H	*L*
Zinc borate	1332-07-6	L	*L*	*H*	*M*	*M*	*H*	L	L		L	L	*H*	*H*	H[R]	*L*

*1 The cited report is a draft for public comment and the front page says **Do not cite or quote**.
*2 Copied from US EPA, 2008
Notes from the cited report:

VL = Very Low hazard **L** = Low hazard **M** = Moderate hazard **H** = High hazard **VH** = Very High hazard –
Endpoints in coloured text (**VL, L, M H**, and **VH**) were assigned based on empirical data.
Endpoints in black italics (*VL, L, M, H,* and *VH*) were assigned using values from predictive models and/or professional judgment.

§ Based on analogy to experimental data for a structurally similar compound.

d This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

♦ Different formulations of the commercial product are available. One of these many formulations has an average MW of ~1,600 and contains significant amounts of lower MW components. These lower MW components are primarily unchanged starting materials that have hazard potentials different than the polymeric flame retardant, as follows: VERY HIGH- Estimated potential for bioaccumulation; HIGH-Experimental concern for acute aquatic toxicity; HIGH-Estimated potential for chronic aquatic toxicity; MODERATE Experimental concern for developmental; and MODERATE-Estimated potential for carcinogenicity, genotoxicity, repeated dose, reproductive, and skin and respiratory sensitization toxicity

¤ This alternative may contain impurities. These impurities have hazard designations that differ from the flame retardant alternative, Confidential Brominated Polymer, as follows, based on experimental data: HIGH for human health, HIGH for aquatic toxicity, VERY HIGH for bioaccumulation, and VERY HIGH for persistence

T This chemical is subject to testing in an EPA consent order.

‡ The highest hazard designation of any of the oligomers with MW <1,000. 0 The highest hazard designation of a representative component of the oligomeric mixture with MWs <1,000.

¥ Phosphonate Oligomer, with a MW range of 1,000 to 5,000, may contain significant amounts of an impurity, depending on the final product preparation. This impurity has hazard designations that differ from the polymeric flame retardant, as follows: MODERATE-Experimental concern for repeated dose, skin sensitization and eye irritation; and HIGH-Experimental concern for reproductive, developmental, acute aquatic toxicity.

R Recalcitrant: Substance is comprised of metallic species that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions.

* Ongoing studies may result in a change in this endpoint

TABLE 45
SCREENING LEVEL HAZARD SUMMARY FOR NON-HALOGENATED PHOSPHOROUS FLAME RETARDANTS USED IN PRINTED CIRCUIT BOARDS (US EPA, 2014B) *1

Chemical	CAS No	Human Health Effects											Aquatic Toxicity		Environ-mental Fate	
		Acute toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Reactive Flame-Retardant Chemicals																
Tetrabromobisphenol A	79-94-7	L	M	L	L♦	M	L	L	L♦		M	L♦	VH	H	H	M
DOPO	35948-25-5	L	M	L	L§	M	M	L	M		M	VL	L	M	H	L
Fyrol PMP	63747-58-0	L	L§	L§	M§	M§	M§	M§	L		L	L	H‡	H‡	VH	H‡
Reactive Flame-Retardant Resins																
D.E.R. 500 Series¥	26265-08-7	L	M	M	M	M	M	M	H		M‡	M‡	L	L	VH	H‡
Dow XZ-92547¥	Confidential	L	M‡	M§	M‡	M‡	M‡	M‡	H	M‡	VL	L	L	H	VH	H‡
Additive Flame-Retardant Chemicals																
Aluminum Diethylphosphinate ¥	225789-38-8	L	L§	L	L	M§	M§	M§	L		L	VL	M	M	HR	L
Aluminum Hydroxide ¥	21645-51-2	L	L§	L	L	M§	M§	M§	L		L	VL	M	M	HR	L
Magnesium Hydroxide ¥	1309-42-8	L	L§	L	L	M§	M§	M§	L		L	VL	M	M	HR	L
Melamine Polyphosphate 1 ¥	15541-60-3	L	M	M	H	M	M	M	L		L	VL	L	L	H	L
Silicon Dioxide (amorphous)	7631-86-9	L ^	L ^	L ^	L	L	L§	H ¤	L		L ^	VL	L	L	HR	L

Notes from the cited report:
VL = Very Low hazard **L** = Low hazard **M** = Moderate hazard **H** = High hazard **VH** = Very High hazard –
Endpoints in coloured text (**VL, L, M H**, and **VH**) were assigned based on empirical data.
Endpoints in black (VL, L, M, H, and VH) were assigned using values from predictive models and/or professional judgement.

♦ TBBPA has been shown to degrade under anaerobic conditions to form bisphenol A (BPA; CASRN 80-05-7). BPA has hazard designations different than TBBPA, as follows: MODERATE (experimental) for reproductive, skin sensitization and dermal irritation.

R Recalcitrant: Substance is comprised of metallic species (or metalloids) that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions.

§ Based on analogy to experimental data for a structurally similar compound.

¤ Concern linked to direct lung effects associated with the inhalation of poorly soluble particles less than 10 microns in diameter.

^ Depending on the grade or purity of amorphous silicon dioxide commercial products, the crystalline form of silicon dioxide may be present. The hazard designations for crystalline silicon dioxide differ from those of amorphous silicon dioxide, as follows: VERY HIGH (experimental) for carcinogenicity; HIGH (experimental) genotoxicity; MODERATE (experimental) for acute toxicity and eye irritation.
¥ Aquatic toxicity: EPA/DfE criteria are based in large part upon water column exposures which may not be adequate for poorly soluble substances such as many flame retardants that may partition to sediment and particulates.

Appendix 2 Modified GreenScreen® Criteria

TABLE 46
MODIFIED GREENSCREEN® CRITERIA FOR HUMAN HEALTH ENDPOINTS

End-point	Information Type	Information Source	List Type	High (H)	Moderate (M)	Low (L)
Carcinogenicity (C)	Data	CLP Criteria & Guidance		CLP Category 1A (Known) or 1B (Presumed) for any route of exposure	CLP Category 2 (Suspected) for any route of exposure or limited or marginal evidence of carcinogenicity in animals (See Guidance)	Adequate data available, and negative studies, no structural alerts, and CLP not classified.
	A Lists	EU CMR (1), harmonised	Authoritative	Category 1 or 2	Category 3	
		EU CMR (2)	Authoritative	Carc 1A or 1B	Carc 2	
		EU H-statements, harmonised	Authoritative	H350 or H350i	H351	
		EU R-phrases	Authoritative	R45 or R49	R40	
		EU SVHC	Authoritative	Reason for inclusion: Carcinogenic		
		IARC	Authoritative	Group 1 or 2A	Group 2B	Group 4
		MAK	Authoritative	Carcinogenic Group 1 or 2	Carcinogenic Group 3, 4, or 5	
		NIOSH-C	Authoritative	Occupational Cancer		
		NTP-RoC	Authoritative	Known or Reasonably Anticipated		
		EPA-C (1986)	Authoritative	Group A, B1 or B2	Group C	Group E
		EPA-C (1996, 1999, 2005)	Authoritative	Known or Likely		Not Likely
	B Lists	EPA-C(1986)	Authoritative	Group D		
		CLP, industry	Screening	Category 1 or 2	Category 3	
		EPA-C (1999)	Authoritative	Suggestive Evidence, but not sufficient to assess human carcinogenic potential		
		EPA-C (2005)	Authoritative	Suggestive evidence of carcinogenic potential		
		IARC	Authoritative	Group 3		

End-point	Information Type	Information Source	List Type	High (H)	Moderate (M)	Low (L)
Mutagenicity/ Genotoxicity (M)	Data	CLP Criteria & Guidance		CLP Category 1A (Known) or 1B (Presumed) for any route of exposure	CLP Category 2 (Suspected) for any route of exposure or limited or marginal evidence of mutagenicity in animals (See Guidance)	Adequate data available and negative studies for both chromosomal aberrations and gene mutations, no structural alerts, and CLP not classified.
	A Lists	EU CMR (1)	Authoritative	Category 1 or 2	Category 3	
		EU CMR (2)	Authoritative	Muta 1A or 1B	Muta 2	
		EU H-statements	Authoritative	H340	H341	
		EU R-phrases	Authoritative	R46	R68	
		EU SVHC	Authoritative	Reason for inclusion: Mutagenic		
	B Lists	MAK	Authoritative	Germ Cell Mutagen 1, 2, or 3a		
		MAK	Authoritative	Germ Cell Mutagen 3b or 5		
Reproductive Toxicity (R)	Data	CLP Criteria & Guidance *Note: CLP Reproductive Toxicity includes both reproductive and developmental effects, while the Green Screen separates them into two distinct hazard endpoints. This classification must be based on reproductive effects alone.*		CLP Category 1A (Known) or 1B (Presumed) for any route of exposure	CLP Category 2 (Suspected) for any route of exposure or limited or marginal evidence of reproductive toxicity in animals (See Guidance)	Adequate data available, and negative, no structural alerts, and CLP not classified.
	A Lists	EU H-statements	Authoritative	H360F, H360FD, H360Fd	H360Df, H361f, H361fd	
		EU R-phrases	Authoritative	R60	R62	
		NTP-OHAaT	Authoritative	Clear Evidence of Adverse Effects - Reproductive		Clear Evidence of No Adverse Effects - Reproductive
	B Lists	NTP-OHAaT	Authoritative	Limited Evidence of Adverse Effects - Reproductive or Some Evidence of Adverse Effects - Reproductive		
						Limited Evidence of No Adverse Effects - Reproductive or Some

End-point	Information Type	Information Source	List Type	High (H)	Moderate (M)	Low (L)
						Evidence of No Adverse Effects - Reproductive
				Insufficient Evidence for a Conclusion - Reproductive Toxicity		
Developmental Toxicity (D)	Data	CLP Criteria & Guidance *Note: CLP Reproductive Toxicity includes both reproductive and developmental effects, while the Green Screen separates them into two distinct hazard endpoints. This classification must be based on developmental effects alone.*		CLP Category 1A (Known) or 1B (Presumed) for any route of exposure	CLP Category 2 (Suspected) for any route of exposure or limited or marginal evidence of developmental toxicity in animals (See Guidance)	Adequate data available, and negative, no structural alerts, and CLP not classified.
	A Lists	EU H-statements	Authoritative	H360FD, H360D, H360Df, or H362	H360Fd, H361d, H361fd	
		EU R-phrases	Authoritative	R61 or R64	R63	
		NTP-OHAaT	Authoritative	Clear Evidence of Adverse Effects - Developmental		Clear Evidence of No Adverse Effects - Developmental
		MAK	Authoritative	Pregnancy Risk Group A or B		
						Pregnancy Risk Group C
				Pregnancy Risk Group D		
		NTP-OHAaT	Authoritative	Limited Evidence of Adverse Effects - Developmental or Some Evidence of Adverse Effects - Developmental		
						Limited Evidence of No Adverse Effects - Reproductive or Some Evidence of No Adverse Effects - Developmental
				Insufficient Evidence for a Conclusion - Developmental Toxicity		
Endocrine Activity (E)	Data	EU ED criteria for prioritisation		Evidence of endocrine disrupting activity in at least one species using intact animals (Category 1 criterion for classification on the EU ED priority list)	At least some in vitro evidence of biological activity related to endocrine disruption (Category 2 criterion for classification on EU ED priority list)	No evidence of endocrine disrupting activity (Category 3a criterion for classification on EU ED priority list)

End-point	Information Type	Information Source	List Type	High (H)	Moderate (M)	Low (L)
		OECD Conceptual Framework		Positive results in in *vivo* tests according to Level 3, 4 and 5 of OECD conceptual framework (ECETOC, 2009)	Positive results in in *vitro* tests according to Level 2 of OECD conceptual framework (ECETOC, 2009)	Negative results in in *vitro* tests according to Level 2 of OECD conceptual framework (ECETOC, 2009)
	A Lists	EU ED	Screening			Category 3a
		EU SVHC	Authoritative	Reason for Inclusion: Endocrine Activity		
	B Lists	EU ED	Screening	Category 1 or 2		
				Category 3b		
		SIN	Screening	Reason for Inclusion: Endocrine Disruptor		

1 Classification according to (DSD) Council Directive 67/548/EEC

2 Classification according to (CLP) Regulation (EC) No 1272/2008

End-point	Information Type	Information Source		List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
Acute Mammalian Toxicity (AT)	Data	CLP Criteria & Guidance			CLP Category 1 or 2 for any route of exposure	CLP Category 3 for any route of exposure	CLP Category 4 for any route of exposure	CLP Category 5 or adequate data available, and negative studies, no structural alerts, and CLP not classified.
		Guidance Values for Animal Data (see CLP for further information)	Oral LD50 (mg/kg)		≤50	>50-300	>300 - 2000	>2000
			Dermal LD50 (mg/kg)		≤200	>200-1000	>1000 - 2000	>2000
			Inhalation-Gas or Vapor LC50(mg/L)		≤2	>2-10	>10 - 20	>20
			Inhalation-Dust/Mist/Fumes LC50 (mg/L)		≤0.5	>0.5-1.0	>1 - 5	>5
	A Lists	EU H-statements		Authoritative	H300, H310, or H330	H301, H311, or H331	H302, H312, or H332	

End-point		Information Type	Information Source		List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
			EU R-phrases		Authoritative	R26, R27 or R28			
			EU R-phrases		Authoritative		R20, R21, or R22		
						R23, R24, or R25			
Systemic Toxicity/Organ Effects (ST)	Single Exposure	Data	CLP Criteria & Guidance			CLP Category 1 Single Exposure for any route of exposure	CLP Category 2 Single Exposure for any route of exposure	CLP Category 3 Single Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and CLP not classified
			CLP Guidance Values for Animal Data (see CLP for further information)	Oral (mg/kg-bw)		≤300	>300-2000		
				Dermal (mg/kg-bw)		≤1000	>1000-2000		
				Inhalation-Gas or Vapor (mg/L/4h)		≤10	>10-20		
				Inhalation-Dust/Mist/Fumes (mg/L/4h)		≤1.0	>1.0-5.0		
		A Lists	EU H-statements		Authoritative	H370	H371	H335	
			EU R-phrases		Authoritative	R39, R39/23, R39/24, or R39/25, R39/26, R39/27, R39/28	R68/20, R68/21, or R68/22,	R37	
	Repeated* Exposure	Data	CLP Criteria & Guidance				CLP Category 1 Repeated Exposure for any route of exposure	CLP Category 2 Repeated Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and CLP not classified
			CLP Guidance Values for Animal Data (see CLP for further information)	Oral (mg/kg-bw/day)			≤10	>10-100	>100
				Dermal (mg/kg-bw/day)			≤20	>20-200	>200
				Inhalation-Gas or Vapor (mg/L/6h/day)			≤0.2	>0.2-1.0	>1.0
				Inhalation-Dust/Mist/Fumes (mg/L/6h/day)			≤0.02	>0.02-0.2	>0.2
			EU H-statements		Authoritative		H372	H373	

End-point		Information Type	Information Source	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
		A Lists	EU R-phrases	Authoritative		R48/23, R48/24, R48/25	R48/20, R48/21, R48/22	
		B Lists	EU R-phrases	Authoritative		R48 "Danger of serious damage to health by prolonged exposure"		
Neurotoxicity	Single Exposure	Data	CLP Criteria Systemic Toxicity/Organ Effects using US EPA Risk Assessment Guidance to define applicable neurotoxic effects.		CLP Category 1 Single Exposure for any route of exposure	CLP Category 2 Single Exposure for any route of exposure	CLP Category 3 Single Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and CLP not classified
		A-Lists	CLP, industry	Screening	Category 1	Category 2	Category 3	"Not Classified"
	Repeated*	Data	CLP Criteria Systemic Toxicity/Organ Effects using US EPA Risk Assessment Guidance to define applicable neurotoxic effects.			CLP Category 1 Repeated Exposure for any route of exposure	CLP Category 2 Repeated Exposure for any route of exposure	Adequate data available, and negative studies, no structural alerts, and CLP not classified
		A Lists	CLP, industry	Screening		Category 1	Category 2	"Not Classified"
	Both	B Lists	EU H-statements	Authoritative			H336	
			EU R-phrases	Authoritative			R67	
Skin Sensitization		Data	GHS Criteria & Guidance			GHS Category 1A (high frequency of occurrence)	GHS Category 1B (low to moderate frequency of occurrence)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
		A Lists	CLP, industry	Screening		Category 1A	Category 1B	"Not Classified"
			MAK	Authoritative		Sensitizing Substances Sh (Skin) or Sah (Respiratory and Skin)		
		B Lists	EU H-statements	Authoritative		H317		
			EU R-phrases	Authoritative		R43		

End-point	Information Type	Information Source	List Type	Very High (vH)	High (H)	Moderate (M)	Low (L)
Respiratory Sensitization (SnR*)	Data	GHS Criteria & Guidance			GHS Category 1A (high frequency of occurrence)	GHS Category 1B (low to moderate frequency of occurrence)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
	A Lists	CLP, industry	Screening		Category 1A	Category 1B	"Not Classified"
		MAK	Authoritative		Sensitizing Substances Sa (Respiratory) or Sah (Respiratory and Skin)		
	B Lists	AOEC	Authoritative		Asthmagen (G)		
					Asthmagen (Rr) and/ or (Rs) and/or (Rrs)		
		EU H-statements	Authoritative		H334		
		EU R-phrases	Authoritative		R42		
Skin Irritation (IrS)	Data	GHS Criteria & Guidance		GHS Category 1 (Corrosive)	GHS Category 2 (Irritant)	GHS Category 3 (Mild irritant)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
		EU H-statements	Authoritative	H314	H315		
		EU R-phrases	Authoritative	R34 or R35	R38		
		CLP, industry	Screening	Category 1	Category 2	Category 3	"Not Classified"
Eye Irritation (IrE)	Data	GHS Criteria & Guidance		GHS Category 1 (Irreversible)	GHS Category 2A (Irritating)	GHS Category 2B (Mildly irritating)	Adequate data available, and negative studies, no structural alerts, and GHS not classified.
	A Lists	EU H-statements	Authoritative	H318	H319	H320	
		EU R-phrases	Authoritative	R41			
		CLP, industry	Screening	Category 1	Category 2A	Category 2B	"Not Classified"
	B Lists	EU R-phrases	Authoritative		R36		

TABLE 47
MODIFIED GREENSCREEN® CRITERIA FOR ENVIRONMENTAL ENDPOINTS

End-point	Information Type	Information Source	List Type	Very High (VH)	High (H)	Moderate (M)	Low (L)	Very Low (VL)
Acute Aquatic Toxicity (AA)	Data	GHS Criteria & Guidance		GHS Category 1	GHS Category 2	GHS Category 3	Sufficient data available and not classified	
		Guidance Values (see GHS for further information) LC_{50} or EC_{50} (mg/L)		≤1	>1 to 10	> 10 to 100	>100	
	A Lists	EU H-statements	Authoritative	H400	H401	H402		
		EU R-phrases	Authoritative	R50	R51	R52		
		CLP (Harmonised; EU)	Authoritative	Category 1	Category 2	Category 3	"Not Classified"	
	B Lists	CLP (Industry classifications)	Screening	Category 1	Category 2	Category 3	"Not Classified"	
Chronic Aquatic Toxicity (CA)	Data	GHS Criteria & Guidance				GHS Category 4		
		Guidance Value (mg/L)		≤0.1	>0.1 to 1.0	> 1.0 to 10	>10	
	A Lists	EU H-statements	Authoritative	H410	H411	H412 or H413		
		EU R-phrases	Authoritative	R50/53	R51/53	R52/53 or R53		
		CLP (Harmonised; EU)	Authoritative	Category 1	Category 2	Category 3	"Not Classified"	
	B Lists	CLP (Industry classifications)	Screening	Category 1	Category 2	Category 3	"Not Classified"	
Persistence (P)	Data	Soil or Sediment		>180 or recalcitrant	>60 to 180	16 to 60	< 16 OR GHS "Rapid degradability"	Meets 10-day window in "Ready Biodegradation Test"
		(1/2 life in days OR Result)						
		Water		> 60 or recalcitrant	> 40 to 60	16 to 40	< 16 OR GHS "Rapid degradability"	Meets 10-day window in "Ready Biodegradation Test"
		(1/2 life in days OR Result)						
		Air		> 5 or recalcitrant	>2 to 5	< 2		

End-point	Information Type	Information Source	List Type	Very High (VH)	High (H)	Moderate (M)	Low (L)	Very Low (VL)
		(1/2 life in days OR Result)						
		Long-Range Environmental Transport			Evidence	Suggestive Evidence		
Bioaccumulation Potential (B)	Data	BAF (Bioaccumulation Factor)		> 5000	> 2000 to 5000	> 500 to 2000	> 100 to 500	≤ 100
		BCF (Bioconcentration Factor)		> 5000	> 2000 to 5000	> 500 to 2000	> 100 to 500	≤ 100
		Log Kow (*Log octanol-water partition coefficient*)		> 5.0*	> 4.5 to 5.0	> 4.0 to 4.5	>3.0 to 4.0	≤ 3
		Monitoring Data (*Presence in humans or wildlife)*			Evidence	Suggestive Evidence		

Remark on bioaccumulation: It should be noted that at very high Log Kow's (i.e. higher than about 7-8) the correlation between Log Kow and BCF is not valid. Thus, in its guidance for PBT assessment ECHA (2012) considers it unlikely that the B-criterion should be fulfilled for substances with Log Kow higher than 10.

Appendix 3 GreenScreen™ for Safer Chemicals - Definitions and Specified Lists

List Type		Definition	Can you modify results?	Level of Confidence
1. Authoritative Lists		**Authoritative lists are those developed by governmental bodies or government recognized expert bodies and include chemicals listed based on results from expert review of test data and scientific literature.**		
	Authoritative A	Each category in the list translates directly to a single level of concern for a single Green Screen hazard endpoint, or a single benchmark. The assigned hazard level cannot be modified using additional data.	NO	High
	Authoritative B	Lists that meet one or more of the following: 1) Each category in the list incorporates a single Green Screen hazard endpoint and does not translate directly to a single level of concern or benchmark; AND/OR 2) Each category in the list refers to more than one Green Screen hazard endpoint. When the range of hazard levels or benchmark levels is narrow, an initial default level of concern may be assigned and may be modified with additional data. When the range is broad, the default hazard level or benchmark is assigned as "unspecified (U)".	YES	High
2. Screening Lists		**Screening lists are either 1) lists developed by authoritative bodies to target chemicals for additional scrutiny and testing and are often generated by models or screening tests; or they are 2) lists developed by non governmental bodies or experts not sanctioned by government.**		
	Screening A	Each category in the list translates directly to a single level of concern for a single Green Screen hazard endpoint, or a single benchmark. The reviewer may modify the level based on weight of evidence.	YES	Low
	Screening B	Lists that meet one or more of the following: 1) Each category in the list incorporates a single Green Screen hazard endpoint and does not translate directly to a single level of concern or benchmark; AND/OR 2) Each category in the list refers to more than one Green Screen hazard endpoint. When the range of hazard levels or benchmark levels is narrow, an initial default level of concern may be assigned and may be modified with additional data. When the range is broad, the default hazard level or benchmark is assigned as "unspecified (U)".	YES	Low

GreenScreen™ for Safer Chemicals Specified Lists Modified by COWI, 3 September 2015						
ID	**Abbreviation**	**CPA List Type**	**Listed in DfE**	**List Name**	**Associated Green Screen Hazard Endpoints**	**URL and/or Reference**
1	AOEC	Authoritative	Yes	Association of Occupational and Environmental Clinics (AOEC) Exposure Code List	Sensitization (respiratory including asthma)	http://www.aoecdata.org/ExpCodeLookup.aspx (accessed 9/14/11)
4	DOT	Authoritative	No	US Department of Transportation Hazardous Materials Regulations	Acute Mammalian Toxicity, Irritation/Corrosivity, Flammability, Reactivity	[Chemicals Listed with Classification-49CFR 172.101] http://ecfr.gpoaccess.gov/cgi/t/text/text-idx?c=ecfr&sid=4011663bcc8928d7775c0b077a36470e&rgn=div8&view=text&node=49:2.1.1.3.8.2.25.1&idno=49 (accessed 9/19/11); [Classification Criteria-49CFR 173] http://ecfr.gpoaccess.gov/cgi/t/text/text-idx?c=ecfr&tpl=/ecfrbrowse/Title49/49cfr173_main_02.tpl (accessed 9/14/11); http://environmentalchemistry.com/yogi/hazmat/placards/ (accessed 9/19/11)
7	EPA - C	Authoritative	Yes	US Environmental Protection Agency (EPA), National Center for Environmental Assessment, Integrated Risk Information System (IRIS) Database	Carcinogenicity	[Search for Cancer Categorization] http://www.epa.gov/ncea/iris/search_human.htm (accessed 9/14/11); [IRIS Database] http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showSubstanceList (accessed 9/14/11)
8	EU CMR (1)	Authoritative	Yes	Regulation on the Classification, Labelling and Packaging of Substances and Mixtures (CLP), EC 1272/2008 and subsequent amendments. Originally published in ECB, Annex I of Directive 67-548-EEC and subsequent amendments/adaptations, known as the Dangerous Substances Directive (DSD) or Directive on Dangerous Substances (DDS).	Carcinogenicity, Mutagenicity/Genotoxicity, Reproductive Toxicity, Developmental Toxicity	[CLP] http://ec.europa.eu/enterprise/sectors/chemicals/classification/index_en.htm (accessed 9/14/11); [DSD] http://ec.europa.eu/environment/chemicals/dansub/home_en.htm (accessed 9/14/11)
9	EU CMR (2)	Authoritative	Yes	Regulation on the Classification, Labelling and Packaging of Substances and Mixtures (CLP), EC 1272/2008 and subsequent	Carcinogenicity, Mutagenicity/Genotoxicity, Reproductive Toxicity, Developmental Toxicity	[CLP] http://ec.europa.eu/enterprise/sectors/chemicals/classification/index_en.htm (accessed 9/14/11)

GreenScreen™ for Safer Chemicals Specified Lists Modified by COWI, 3 September 2015						
ID	**Abbreviation**	**CPA List Type**	**Listed in DfE**	**List Name**	**Associated Green Screen Hazard Endpoints**	**URL and/or Reference**
				amendments. [Conversion of CMR list from 67-548- EEC(Categories 1-3) to GHS Categories (Category 1A, 1B, 2)]		
10	EU ED	Screening	No	European Union Priority List of suspected endocrine disruptors (prioritized for further testing). Chemicals prioritized by the European Union for testing for endocrine disruption. DHI. 2007. Study on Enhancing the Endocrine Disruptor Priority List with a Focus on Low Production Volume Chemicals.	Potential Endocrine Disruptor	[Website] http://ec.europa.eu/environment/endocrine/strategy/substances_en.htm#priority_list (accessed 9/14/11); [Report] http://ec.europa.eu/environment/endocrine/documents/final_report_2007.pdf (accessed 9/23/11)
11	EU H-Statements	Authoritative	Yes	European Union List of Chemicals and their assigned GHS Hazard Statement is included in the Regulation on the Classification, Labelling and Packaging of Substances and Mixtures (CLP), EC 1272/2008 and subsequent amendments.	Carcinogenicity, Mutagenicity/Genotoxicity, Reproductive Toxicity, Developmental Toxicity, Acute Mammalian Toxicity, Systemic Toxicity/Organ Effects, Neurotoxicity, Sensitization, Irritation/Corrosivity, Flammability, Reactivity, Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Ecotoxicity	[CLP] http://ec.europa.eu/enterprise/sectors/chemicals/classification/index_en.htm (accessed 8/1/11) [ESIS Database-CLP/GHS] http://esis.jrc.ec.europa.eu/index.php?PGM=cla (accessed 10/4/11)
12	EU PBT	Authoritative	No	European Union, European Chemicals Bureau, European Chemical Substances Information System (ESIS) PBT list	PBT and vPvB: Persistence, Bioaccumulation and any of the following: ecotox and/or human tox	[ESIS Database-PBT] http://esis.jrc.ec.europa.eu/index.php?PGM=pbt (accessed 9/14/11)
13	EU R-Phrases	Authoritative	Yes	EU Risk-Phrases published in the Regulation on the Classification, Labelling and Packaging of Substances and Mixtures (CLP), EC 1272/2008 and subsequent amendments. Originally published in ECB, Annex	Carcinogenicity, Mutagenicity/Genotoxicity, Reproductive Toxicity, Developmental Toxicity, Acute Mammalian Toxicity, Systemic Toxicity/Organ Effects, Neurotoxicity, Sensitization, Irritation/Corrosivity, Flamma-	[CLP] http://ec.europa.eu/enterprise/sectors/chemicals/classification/index_en.htm (accessed 9/14/11); [DSD] http://ec.europa.eu/environment/chemicals/dansub/home_en.htm (accessed 9/14/11)

GreenScreen™ for Safer Chemicals Specified Lists Modified by COWI, 3 September 2015						
ID	**Abbreviation**	**CPA List Type**	**Listed in DfE**	**List Name**	**Associated Green Screen Hazard Endpoints**	**URL and/or Reference**
				I of Directive 67-548-EEC and subsequent amendments/adaptations, known as the Dangerous Substances Directive (DSD) or Directive on Dangerous Substances (DDS).	bility, Reactivity, Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Ecotoxicity	
14	EU SVHC	Authoritative	No	European Union Substances of Very High Concern Authorization List (Note: Inclusion of the Candidate List to be determined.)	Carcinogenicity; Mutagenicity/Genotoxicity; Reproductive Toxicity; Developmental Toxicity; PBT: Persistence, Bioaccumulation, and ecotoxicity and/or human toxicity; vPvB: very persistent and very bioaccumulative, other serious concerns (e.g. Endocrine Activity)	http://echa.europa.eu/consultations/authorisation/svhc/svhc_cons_en.asp (accessed 9/14/11)
16	IARC	Authoritative	Yes	International Agency for Research on Cancer (IARC), Agents Reviewed by the IARC Monographs	Carcinogenicity	[List of Classifications] http://monographs.iarc.fr/ENG/Classification/index.php (accessed 9/14/11); [Monographs] http://monographs.iarc.fr/ (accessed 9/14/11)
17	MAK	Authoritative	No	MAK Commission of Germany; Occupational Toxicants and MAK Values: Annual Thresholds and Classifications for the Workplace	Carcinogenicity, Reproductive and Developmental Toxicity including Developmental Neurotoxicity, Sensitization	[DFG Working Group Chairs] http://www.dfg.de/en/dfg_profile/statutory_bodies/senate/health_hazards/structure/working_groups/derivation_mak/index.html (accessed 10/4/11) 1) Professor Dr. Andrea Hartwig Karlsruher Institut für Technologie (KIT): (andrea.hartwig@kit.edu, phone: +49 721 608 47645) 2) Prof. Dr. med. Hans Drexler, Universität Erlangen- Nürnberg: (Hans.Drexler@ipasum.uni-erlangen.de, phone: +49 9131 85-22312); [Publication] List of MAK and BAT Values 2011: Maximum Concentrations and Biological Tolerance Values at the Workplace, Report 47 Deutsche Forschungsgemeinschaft (DFG) (Editor) ISBN: 978-3-527-33061-4 Paperback; 292 pages; December 2011 [Purchase from Wiley] http://www.wiley.com/WileyCDA/WileyTitle/productCd-

GreenScreen™ for Safer Chemicals Specified Lists Modified by COWI, 3 September 2015						
ID	**Abbreviation**	**CPA List Type**	**Listed in DfE**	**List Name**	**Associated Green Screen Hazard Endpoints**	**URL and/or Reference**
						3527330615.html (accessed 9/23/11)
18	NIOSH-C	Authoritative	Yes	National Institute of Occupational Safety and Health Carcinogen List	Carcinogenicity	http://www.cdc.gov/niosh/topics/cancer/npotocca.html (accessed 9/19/11)
26	Stockholm	Authoritative	No	United Nations Environment Programme (UNEP), Stockholm Convention Secretariat Stockholm Convention on Persistent Organic Pollutants (POPs)	Persistence, Bioaccumulation and any of the following: ecotox and/or human tox	http://chm.pops.int/Convention/ThePOPs/tabid/673/language/en-US/Default.aspx (accessed 9/19/11)
28	TRI PBT	Authoritative	No	US Environmental Protection Agency (EPA), Toxics Release Inventory (TRI) Program, "TRI PBT Chemical List"	Persistence, Bioaccumulation, Acute Aquatic Toxicity	http://www.epa.gov/tri/trichemicals/pbt%20chemicals/pbt_chem_list.htm (accessed 9/19/11)
35	SIN	Screening	No	International Chemical Secretariat (ChemSec) Substitute it Now (SIN) List; SIN List 2.0 Available 2011	Carcinogenicity; Mutagenicity/Genotoxicity; Reproductive Toxicity; Developmental Toxicity; PBT: Persistence, Bioaccumulation, and ecotoxicity and/or human toxicity; vPvB: very persistent and very bioaccumulative, other serious concerns (e.g. Endocrine Activity)	http://www.chemsec.org/list/sin-database (accessed 9/19/11)
36	VwVwS	Screening	No	German Federal Environment Agency, Administrative Regulation on the Classification of Substances hazardous to waters into Water Hazard Classes (Verwaltungsvorschrift wassergefahrdende Stoffe - VwVwS)	Any combination of the following: Acute Toxicity, Systemic Toxicity/Organ Effects, Carcinogenicity, Reproductive Toxicity, Developmental Toxicity, Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Persistence, Bioaccumulation. Any combination results in Classification of 0-3.	[Database of Chemicals and Classifications] http://webrigoletto.uba.de/rigoletto/public/searchRequest.do;jsessionid=88A1AE1DEE0223CFE7DD76B71FE35F67?event=request (accessed 9/19/11); [Information] http://webrigoletto.uba.de/rigoletto/public/downloadShow.do?event=show&rubric=5; http://www.umweltbundesamt.de/wgs-e/wgs- down.htm#a1-2 (accessed 9/19/11);

1 Classification according to (DSD) Council Directive 67/548/EEC

*Note: The Green Screen List of Lists includes all publically accessible published lists of chemicals classified using the Globally Harmonized System of Classification and Labeling and published by an authoritative governmental organization of a country. Country-specific GHS lists may be published by specifying GHS Categories or GHS H- statements for a group of chemicals. As of July 2011, the countries with published lists include the European Union, Japan, Korea, and New Zealand.

Appendix 4 GreenScreen™ for List Translator – Benchmark 1 only + Possible Benchmark 1

GreenScreenTM List Translator Benchmark 1 Lists Only Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			GreenScreen® List Translator					
ID	List	List Category	Green Screen Hazard	List Type	A or B	Hazard Range	Display in Hazard Box (See Notes)	Benchmark Score
20	EPA-C	(1986) Group A - Human Carcinogen	Carcinogenicity	Authoritative	A	H	**H**	**1**
21	EPA-C	(1986) Group B1 - Probably human carcinogen	Carcinogenicity	Authoritative	A	H	**H**	**1**
22	EPA-C	(1986) Group B2 - Probably human carcinogen	Carcinogenicity	Authoritative	A	H	**H**	**1**
23	EPA-C	(1996) Known/likely human carcinogen	Carcinogenicity	Authoritative	A	H	**H**	**1**
24	EPA-C	(1999, 2005) Carcinogenic to humans	Carcinogenicity	Authoritative	A	H	**H**	**1**
25	EPA-C	(1999, 2005) Likely to be carcinogenic to humans	Carcinogenicity	Authoritative	A	H	**H**	**1**
32	EU CMR (1)	Carcinogen Category 1: "known"	Carcinogenicity	Authoritative	A	H	**H**	**1**
33	EU CMR (1)	Carcinogen Category 2: "should be considered carcinogenic to humans"	Carcinogenicity	Authoritative	A	H	**H**	**1**
34	EU CMR (1)	Mutagen Category 1: "Substances known to be mutagenic to man"	Mutagenicity/Genotoxicity	Authoritative	A	H	**H**	**1**
35	EU CMR (1)	Mutagen Category 2: "Substances which should be regarded as if they are mutagenic to	Mutagenicity/Genotoxicity	Authorita-	A	H	**H**	**1**

GreenScreenTM List Translator Benchmark 1 Lists Only Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			**GreenScreen® List Translator**					
ID	**List**	**List Category**	**Green Screen Hazard**	**List Type**	**A or B**	**Hazard Range**	**Display in Hazard Box (See Notes)**	**Benchmark Score**
		man"		tive				
38	EU CMR (2)	Carc 1A	Carcinogenicity	Authorita-tive	A	H	**H**	**1**
39	EU CMR (2)	Carc 1B	Carcinogenicity	Authorita-tive	A	H	**H**	**1**
40	EU CMR (2)	Muta 1A	Mutagenicity/Genotoxicity	Authorita-tive	A	H	**H**	**1**
41	EU CMR (2)	Muta 1B	Mutagenicity/Genotoxicity	Authorita-tive	A	H	**H**	**1**
48	EU H-statem	H360D "May damage the un-born child."	Developmental Toxicity	Authorita-tive	A	H	**H**	**1**
49	EU H-statem	H360FD "May damage fertility. May damage the unborn child."	Developmental Toxicity	Authorita-tive	A	H	**H**	**1**
50	EU H-statem	H360Df "May damage the unborn child. Suspected of damaging fertility."	Developmental Toxicity	Authorita-tive	A	H	**H**	**1**
54	EU H-statem	H350 "May cause cancer "	Carcinogenicity	Authorita-tive	A	H	**H**	**1**
55	EU H-statem	H350i "May cause cancer by inhalation"	Carcinogenicity	Authorita-tive	A	H	**H**	**1**
78	EU H-statem	H340 "May cause genetic de-fects "	Mutagenicity/Genotoxicity	Authorita-tive	A	H	**H**	**1**
88	EU H-statem	H362 "May cause harm to breast-fed children."	Developmental Toxicity	Authorita-tive	A	H	**H**	**1**
89	EU H-statem	H360F "May damage fertility."	Reproductive Toxicity	Authorita-tive	A	H	**H**	**1**
		H360FD "May damage fertility.						

GreenScreenTM List Translator Benchmark 1 Lists Only Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			GreenScreen® List Translator					
ID	List	List Category	Green Screen Hazard	List Type	A or B	Hazard Range	Display in Hazard Box (See Notes)	Benchmark Score
90	EU H-statem	May damage the unborn child."	Reproductive Toxicity	Authoritative	A	H	**H**	**1**
91	EU H-statem	H360Fd "May damage fertility. Suspected of damaging the unborn child."	Reproductive Toxicity	Authoritative	A	H	**H**	**1**
96	EU R-phrases	R45 “May cause cancer”	Carcinogenicity	Authoritative	A	H	**H**	**1**
118	EU R-phrases	R49 “May cause cancer by inhalation”	Carcinogenicity	Authoritative	A	H	**H**	**1**
122	EU R-phrases	R46 “May cause heritable genetic damage“	Mutagenicity/Genotoxicity	Authoritative	A	H	**H**	**1**
137	EU R-phrases	R60 “May impair fertility”	Reproductive Toxicity	Authoritative	A	H	**H**	**1**
138	EU R-phrases	R61 “May cause harm to the unborn child”	Developmental Toxicity	Authoritative	A	H	**H**	**1**
142	EU R-phrases	R64 "May cause harm to breastfed babies"	Developmental Toxicity	Authoritative	A	H	**H**	**1**
148	EU SVHC	Reason for inclusion: Carcinogenic	Carcinogenicity	Authoritative	A	H	**H**	**1**
149	EU SVHC	Reason for inclusion: Mutagenic	Mutagenicity/Genotoxicity	Authoritative	A	H	**H**	**1**
150	EU SVHC	Reason for Inclusion: Other concern - Endocrine Activity	Endocrine Activity	Authoritative	A	H	**H**	**1**
153	IARC	Group 1: Agent is carcinogenic to humans	Carcinogenicity	Authoritative	A	H	**H**	**1**

GreenScreenTM List Translator Benchmark 1 Lists Only Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			**GreenScreen® List Translator**					
ID	**List**	**List Category**	**Green Screen Hazard**	**List Type**	**A or B**	**Hazard Range**	**Display in Hazard Box (See Notes)**	**Benchmark Score**
154	IARC	Group 2A: Agent is probably carcinogenic to humans	Carcinogenicity	Authoritative	A	H	**H**	**1**
158	MAK	Carcinogenic Group 1	Carcinogenicity	Authoritative	A	H	**H**	**1**
159	MAK	Carcinogenic Group 2	Carcinogenicity	Authoritative	A	H	**H**	**1**
174	NIOSH-C	Occupational Cancer	Carcinogenicity	Authoritative	A	H	**H**	**1**
8	Stockholm	POP	PBT [Persistence, Bioaccumulation and any of the following: Ecotoxicity and/or Human Toxicity (Human Health Effects)]	Authoritative	A	U	**Mult***	**1**
9	WA PBT	PBT	PBT [Persistence, Bioaccumulation and any of the following: Ecotoxicity and/or Human Toxicity (Human Health Effects)]	Screening	A	U	*Mult**	**1**
10	EPA PBT	PBT	PBT [Persistence, Bioaccumulation and any of the following: Ecotoxicity, Carcinogenicity, Mutagenicity, Reproductive Toxicity, Developmental Toxicity, Neurotoxicity, Other chronic effects, or effects from site releases]	Authoritative	A	U	**Mult***	**1**
11	EU PBT	PBT	PBT [Persistence, Bioaccumulation and any of the following: Ecotoxicity and/or Human Toxicity (Human Health Effects)]	Authoritative	A	U	**Mult***	**1**
11.5	EU PBT	POP	Persistent Organic Pollutant [Persistence, Bioaccumulation and any of the following: Ecotoxicity and/or Human Toxicity (Human Health Effects)]	Authoritative	A	U	**Mult***	**1**
12	TRI PBT	PBT	PBT [Persistence, Bioaccumulation, and Acute Aquatic Toxicity]	Authoritative	A	U	**Mult***	**1**
13	OSPAR	PBT	PBT [Persistence, Bioaccumulation, and any of the following: Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Carcinogenicity, Mutagenicity, Reproductive Toxicity, Developmental Toxicity, Systemic Toxicity/Organ Effects repeated exposure)]	Authoritative	A	U	**Mult***	**1**
			PBT [Persistence, Bioaccumulation, and any of the following:					

GreenScreenTM List Translator Benchmark 1 Lists Only Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			**GreenScreen® List Translator**					
ID	**List**	**List Category**	**Green Screen Hazard**	**List Type**	**A or B**	**Hazard Range**	**Display in Hazard Box (See Notes)**	**Benchmark Score**
14	EU SVHC	Reason for Concern: PBT	Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Carcinogenicity, Mutagenicity, Reproductive Toxicity, Developmental Toxicity]	Authoritative	A	U	**Mult***	**1**
20	EU CMR (2)	Repr 1A	Reproductive and/or Developmental Toxicity	Authoritative	B	H (R and/or D)	*Mult**	**1**
21	EU CMR (2)	Repr 1B	Reproductive and/or Developmental Toxicity	Authoritative	B	H (R and/or D)	*Mult**	**1**
22	EU CMR (1)	Reproduction Category 1: “known” to impair fertility in humans or cause developmental toxicity in humans”	Reproductive and/or Developmental Toxicity	Authoritative	B	H (R and/or D)	*Mult**	**1**
23	EU CMR (1)	Reproduction Category 2: “should be regarded as if” they impair fertility to humans or cause developmental toxicity to humans”	Reproductive and/or Developmental Toxicity	Authoritative	B	H (R and/or D)	*Mult**	**1**
24	EU SVHC	Reason for inclusion: Toxic for reproduction	Reproductive and/or Developmental Toxicity	Authoritative	B	H (R and/or D)	*Mult**	**1**
25	EU H-statement	H360 (with any combo of letters or no letters) "May damage fertility or the unborn child <state specific effect if known > <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard"	Reproductive and/or Developmental Toxicity	Screening	B	H (R and/or D)	*Mult**	**1**

GreenScreenTM List Translator Benchmark 1 Lists Only Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			**GreenScreen® List Translator**					
ID	**List**	**List Category**	**Green Screen Hazard**	**List Type**	**A or B**	**Hazard Range**	**Display in Hazard Box (See Notes)**	**Benchmark Score**
38	EU PBT	vPvB	vPvB [Persistence, Bioaccumulation]	Authorita-tive	A	U	**Mult***	**1**
39	EU SVHC	Reason for Concern: vPvB	vPvB [Persistence, Bioaccumulation]	Authorita-tive	A	U	**Mult***	**1**
40	SIN	CMR	One or more of the following: Carcinogenicity, Mutagenicity, Reproductive Toxicity, Developmental Toxicity.	Screening	A	U	*Mult**	**1**
41	SIN	PBT	PBT [Persistence, Bioaccumulation and any of the following: Ecotoxicity and/or Human Toxicity (Human Health Effects)]	Screening	A	U	*Mult**	**1**
42	SIN	vPvB	Persistence and Bioaccumulation	Screening	A	U	*Mult**	**1**

1 Classification according to (DSD) Council Directive 67/548/EEC

2 Classification according to (CLP) Regulation (EC) No 1272/2008

GreenScreen™ ListTranslator Possible Benchmark 1 (Benchmark 1 or 2 Lists Only) Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			**GreenScreen® List Translator**					
ID	**List**	**List Category**	**Green Screen Hazard**	**List Type**	**A or B**	**Hazard Range**	**Display in Hazard Box (See Notes)**	**Benchmark Score**
45	EU ED	Category 1 ("at least one in-vivo study providing *clear evide*nce for endocrine disruption in at least one species using intact animals"),	Endocrine Activity	Screening	B	H or M	*H or M (3)*	**Possible BM 1**
46	EU ED	Category 2 ("Potential for endocrine disruption. *In-vitro* data indicating potential for endocrine disruption in intact organisms. Also includes effects *in- vivo* that may, or may not, be ED- mediated.")	Endocrine Activity	Screening	B	H or M	*H or M (3)*	**Possible BM 1**
161	MAK	Germ Cell Mutagen 2	Mutagenicity/Genotoxicity	Authoritative	B	H or M	*H or M (3)*	**Possible BM 1**
162	MAK	Germ Cell Mutagen 3a	Mutagenicity/Genotoxicity	Authoritative	B	H or M	*H or M (3)*	**Possible BM 1**
165	MAK	Pregnancy Risk Group A	Developmental Toxicity	Authoritative	B	H or M	*H or M (3)*	**Possible BM 1**
166	MAK	Pregnancy Risk Group B	Developmental Toxicity	Authoritative	B	H or M	*H or M (3)*	**Possible BM 1**
196	SIN	Reason for Inclusion: Endocrine Disruptor	Endocrine Activity	Screening	B	H or M	*H or M (3)*	**Possible BM 1**
197	TEDX	Listed on the TEDX List of Potential Endocrine Disruptors	Endocrine Activity	Screening	B	H or M	*H or M (3)*	**Possible BM 1**
31	EU R-phrases	R50/53 "Very Toxic to Aquatic Organisms, May cause long-term adverse effects in the aquatic environment"	T & P and/or B [Chronic Aquatic Toxicity and sometimes Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	Authoritative	B	U	*Mult**	**Possible BM 1**
32	EU R-phrases	R51/53 Toxic to Aquatic Organisms, May cause long-term adverse effects in the aquatic environment	T & P and/or B [Chronic Aquatic Toxicity and sometimes Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	Authoritative	B	U	*Mult**	**Possible BM 1**

GreenScreen™ ListTranslator Possible Benchmark 1 (Benchmark 1 or 2 Lists Only) Modified by COWI, 3 September 2015								
GreenScreen® Supporting List Information			**GreenScreen® List Translator**					
ID	**List**	**List Category**	**Green Screen Hazard**	**List Type**	**A or B**	**Hazard Range**	**Display in Hazard Box (See Notes)**	**Benchmark Score**
33	EU H-statement	H410 "Very toxic to aquatic life with long lasting effects."	T & P and/or B [(Chronic Aquatic Toxicity and sometimes Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	Screening	B	U	*Mult**	**Possible BM 1**
34	EU H-statement	H411 "Toxic to aquatic life with long lasting effects."	T & P and/or B [(Chronic Aquatic Toxicity and sometimes Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	Screening	B	U	*Mult**	**Possible BM 1**
44	VwVwS	Class 2-"hazard to waters"	Any combination of the following: Acute Mammalian Toxicity, Systemic Toxicity/Organ Effects, Carcinogenicity, Reproductive Toxicity, Developmental Toxicity, Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Persistence, Bioaccumulation.	Screening	B	U	*Mult**	**Possible BM 1**
45	VwVwS	Class 3-"severe hazard to waters"	Any combination of the following: Acute Mammalian Toxicity, Systemic Toxicity/Organ Effects, Carcinogenicity, Reproductive Toxicity, Developmental Toxicity, Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Persistence, Bioaccumulation.	Screening	B	U	*Mult**	**Possible BM 1**
160	MAK	Germ Cell Mutagen 1	Mutagenicity/Genotoxicity	Authoritative	B	H or M	*H or M (3)*	**Possible BM 1**

Appendix 5 Phenol, isobutylenated, phosphate, CAS No. 68937-40-6

NOTE: Data from REACH registration dossiers are mostly on commercial substances such as Phosflex, Furquel etc.. According to REACH registration, phenol, isobutylenated, phosphate is made up of four different constituents: p-t-butylphenyl diphenyl phosphate, bis(p-t-butylphenyl) phenyl phosphate, tris(p-tert-butylphenyl) phosphate and triphenyl phosphate.

Regarding the data from Brooke et al. 2009 it is stated that the assessment covers the commercial substances tertbutylphenyl diphenyl phosphate (CAS No. 56803-37-3/EC no. 260-391-0) and Phenol, isobutylated, phosphate (3:1) (Cas no. 68937-40-6/EC no. 273-065-8). It is furthermore stated in Brooke et al. (2009) that CAS No. 220352-35-2 (butylated triphenyl phosphate) is also used by European suppliers of this substance, although this is not listed on the European Inventory of Existing Commercial Chemical Substances (EINECS). Akzo Nobel data is for Butylated triphenyl phosphate (CAS No. 220352-35-2) and t-butylphenyl diphenyl phosphate is mentioned as a synonym.

A notified classification is available for Phenol, isobutylenated, phosphate (3:1); Aquatic Chronic 1 (H410; 1 notifier) and Aquatic Chronic 3 (H412; 1 notifier).

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0			
Property/Endpoint	**Data**	**Reference**	**Comments**
Physical/chemical properties			
Melting Point (°C)	- 21 °C (for tertbutylphenyl diphenyl phosphate) (measured)	REACH registration data; Brooke et al. 2009.	Reported in a secondary source. Reliable, however, data is for tertbutylphenyl diphenyl phosphate (EC no. 260-391-0) Melting point is reported as pouring point.
Boiling Point (°C)	260-420 °C for commercial products of tertbutylphenyl diphenyl phosphate (measured)	Brooke et. al. 2009	Reported in a secondary source (review)
	> 400 °C for the commercial product Phosflex 61B (t-Butylated triphenyl phosphate ester) (measured)	REACH registration data	Reported in a secondary source. Experimental value, reliable (standardised guidelines)
Vapour Pressure (Pa)	3.24 x 10^{-4} Pa at 20 °C for the commercial product Phosflex 71B (t-Butylated diphenyl phosphate) (measured)	REACH registration data	Reported in a secondary source. Experimental value, reliable (standardised guidelines, GLP compliance)
	4.2 x 10^{-5} Pa at 25 °C (specific test compound not specified,	REACH registration data	Reported in a secondary source. Experi-

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0			
Property/Endpoint	**Data**	**Reference**	**Comments**
	i.e. commercial product name) (measured)		mental value, reliable (standardised guidelines)
	7.8 × 10^{-5} Pa at 20°C and 1.5×10^{-4} Pa at 25°C for tertbutylphenyl diphenyl phosphate (estimated)	Brooke et al. 2009	Reported in a secondary source (review). Estimated based on information on boiling points at reduced pressures and vapour pressure at elevated temperature from different data sources. Estimates are based on mathematical modelling.
	1.08 x 10^{-3} Pa at 20°C for the commercial product Phosflex 61B (t-Butylated triphenyl phosphate ester)	Akzo Nobel, 2004	Reported in a secondary source.
Water Solubility (mg/L)	3.2 mg/L at room temperature (test substance: tertbutylphenyl diphenyl phosphate along with triphenyl phosphate and bis(tertbutylphenyl) phenyl phosphate) (measured)	Brooke et al. 2009	Reported in a secondary source (review), test substance close to similar to phenol, isobutylenated, phosphate
	0.04 mg/L (test substance tertbutylphenyl diphenyl phosphate) (measured)	Akzo Nobel, 2004	Reported in a secondary source, standardised guideline
	0.009 mg/L at 25°C (estimated, based on a log kow of 6.61)	Brooke et al. 2009	Reported in a secondary source (review). Data estimated using the Syracuse Research Corporation WSKOW version 1.30 software
Log Kow	5.12 (test substance: tertbutylphenyl diphenyl phosphate along with triphenyl phosphate and bis(tertbutylphenyl) phenyl phosphate) (measured)	Brooke et al. 2009	Reported in a secondary source (review). Test substance close to similar to phenol, isobutylenated, phosphate
	6.61 (for tertbutylphenyl diphenyl phosphate (estimated on the basis of the compound structure)	Brooke et al. 2009	Data estimated using the Syracuse Research Corporation WSKOW version 1.30 software
	Weighted average log Kow (Pow) 4.86 for the commercial	REACH registration data	Reported in a secondary source. Weighted

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0			
Property/Endpoint	**Data**	**Reference**	**Comments**
	product Phosflex 71B t-Butylated diphenyl phosphate) (calculated based on measured data)		average is based on log Kow values for the two main mixture components (TTP and C4)
	4.85 for the commercial product Phosflex 61B (measured data)	Akzo Nobel, 2004	Reported in a secondary source.
pKa	The pKa of the leaving phenol group is around 10, and a similar value would be expected for the tertbutylphenyl leaving group (estimated)	Brooke et al. 2009	Reported in a secondary source (review).

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0				
Property/Endpoint		**Data**	**Reference**	**Comments**
Human health effects				
Toxicokinetics		**No data**		
Dermal absorption *in vitro*		No data available	Brooke et al. 2009	
Absorption, Distribution, Metabolism & Excretion	Oral, dermal or inhaled	No data available	Brooke et al. 2009	
	Other	No data available	Brooke et al. 2009	
Acute mammalian toxicity		**LOW:** Oral LD50 in rats and mice is >5,000 mg/kg and the dermal LD50 in rabbits is >2,000 mg/kg in tests with a commercial products containing 75-80 % w/w tertbutylphenyl diphenyl phosphate, 20-25 % w/w triphenyl phosphate CAS No. 115-86-6.		
Acute lethality	Oral	Rat, oral LD_{50} > 5000 mg/kg bw for commercial product Phosflex 51B ((75-80 % w/w tertbutylphenyl diphenyl phosphate, 20-25 % w/w triphenyl phosphate CAS No. 115-86-6)	Akzo Nobel, 2004	Reported in a secondary source. Guideline EPA OTS 798.1175 , no GLP compliance. Reliability 1 according to Akzo Nobel.
		Rat, oral LD_{50} > 5000 mg/kg bw for commercial product Fyrquel LT for male and female rats	REACH registration data	Reported in a secondary source. Non-GLP study according to methodology comparable to OECD guideline 401. Several minor deviations from guideline. Reliability 2
	Dermal	Rabbit, dermal LD_{50} > 2000 mg/kg bw for commercial product Phosflex 72B for male and female rabbits	REACH registration data	Reported in a secondary source. Non-GLP study according to methodology comparable to OECD guideline 402. Several minor deviations from guideline. Reliability 2
		Rabbit, dermal LD_{50} > 2000 mg/kg bw for commercial product Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate CAS No. 115-86-6) for male and female rabbits	Akzo Nobel, 2004	Reported in a secondary source. Guideline EPA OTS 798.1100, no GLP compliance. Reliability 1 according to Akzo Nobel.
	Inhalation	Rat, inhalation LC_{50} > 3.1 mg/l (highest dose tested) for	Akzo Nobel, 2004, Brooke	Reported in a secondary source. Guide-

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0				
Property/Endpoint		**Data**	**Reference**	**Comments**
		commercial product Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate CAS No. 115-86-6) for male and female rats	et al. 2009	line OPPTS 870.1300, no GLP compliance. Reliability 1 according to Akzo Nobel.
		Male rats, inhalation LC_{50} > 0.4 mg/l (only dose tested) of vaporized test material for, 6h for the commercial product Santicizer 154. No mortality occurred.	REACH registration data	Reported in a secondary source. Early GLP, but no guideline followed. Reliability 2
Carcinogenicity		**No data**		
	QSAR results from the literature (e.g. Danish QSAR database)	No data located		
	Carcinogenicity (Rat and Mouse)	No data available	Brooke et al. 2009	
	Combined Chronic Toxicity/Carcinogenicity	No data available	Brooke et al. 2009	
	Other	No data located		
Genotoxicity		**LOW:** A commercial product containing 75-80 % w/w tertbutylphenyl diphenyl phosphate, 20-25 % w/w triphenyl phosphate CAS No. 115-86-6 was not mutagenic in bacteria or mammalian cells in vitro and did not cause chromosomal aberrations or sister chromatide exchanges in vitro.		
	Gene Mutation *in vitro*	Commercial product Phosflex 51B: Negative, Ames Assay in *Salmonella typhimurium* strains TA-1535, TA-1537, TA-1538, TA-98, and TA-100, with and without metabolic activation.	Akzo Nobel, 2004; Brooke et al.2009	Reported in a secondary source.
		Commercial product Phosflex 51B: Negative, forward mutation assay in mouse lymphoma L5178Y cells in the presence and absence of an induced rat live metabolic activating system	Akzo Nobel, 2004; Brooke et al.2009	Reported in a secondary source.
	Gene Mutation *in vivo*	No data available	Brooke et al. 2009	
	Chromosomal Aberrations *in vitro*	Commercial product Phosflex 51B: Did not induce chromo-	Akzo Nobel, 2004; Brooke	Reported in a secondary source.

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0				
Property/Endpoint		**Data**	**Reference**	**Comments**
		somal aberrations or sister chromatid exchanges in the mouse lymphoma cytogenetic assay, in the presence and absence of an induced rat liver metabolic activating system.	et al.2009	
	Chromosomal Aberrations *in vivo*	No data available	Brooke et al. 2009	
	DNA Damage and Repair	No data located		
	Other	No data located		
Reproductive effects		**LOW:** Based on a rat oral reproductive/developmental NOAEL = 1000 mg/kg-bw/day for reproductive effects (highest dose tested).		
	Reproduction/Developmental Toxicity Screen	Reproductive/developmental oral gavage study in rats (14 days pre-mating, 14 days during mating and through gestation and lactation (approx. 8 weeks in total), 12/sex/group, test dose: 0, 50, 250 or 1,000 mg/kg bw/day of the commercial product Phosflex 61B. Based on the lack of parental and foetal toxicity, the no observed adverse effects level (NOAEL) for this study was greater than 1,000 mg/kg bw/day.	Akzo Nobel, 2004; Brooke et al. 2009	Reported in a secondary source (review). The study was conducted to OECD 421 and EPA OPPTS 870.3550 test guidelines and to GLP
	Continuous breeding study	A modification of the National Toxicology Program's (NTP) Continuous Breeding Protocol was conducted in F344 rats exposed orally to 0, 600, 1000, or 1700 mg/kg butylated triphenyl phosphate-based hydraulic fluid for 135 days. LOAEL = 1000 mg/kg-bw/day (based on multiple effects in males and females) NOAEL = 600 mg/kg-bw/day	US EPA 2008	Reported in a secondary source.
	Combined Repeated Dose with Reproduction/Developmental Toxicity Screen	No data located		
	Reproduction and Fertility Effects	No data located		
	Other	No data located		
Developmental effects		**LOW:** Based on a rat oral reproductive/developmental NOAEL = 1000 mg/kg-bw/day for developmental effects (highest dose tested). There were no data located for the developmental neurotoxicity endpoint. Decreased cholinesterase activity in pregnant lab animals has		

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0				
Property/Endpoint		**Data**	**Reference**	**Comments**
		been shown to have a negative impact on foetal brain development. As a result, there is uncertain potential for developmental neurotoxicity for this substance.		
	Reproduction/Developmental Toxicity Screen	Reproductive/developmental oral gavage study (14 days pre-mating, 14 days during mating and through gestation and lactation (approx. 8 weeks in total), 12/sex/group, test dose: 0, 50, 250 or 1,000 mg/kg bw/day of the commercial product Phosflex 61B. No effect on litter size or the number of live pubs on postnatal days 0 and 4.	Akzo Nobel, 2004; Brooke et al. 2009	Reported in a secondary source. The study was conducted to OECD 421 and EPA OPPTS 870.3550 test guidelines and to GLP
		21 day teratogenicity study: 30 pregnant rats/group received either 0, 100,400, or 1000 mg/kg/day of Phosflex 5 1 B by oral gavage from gestation day 6 through gestation day 20. A significant dose-related increase in absolute and relative liver weights was observed in all treatment groups, which was considered by the authors to be an adaptive response (enzyme induction) rather than due to toxicity of the compound, although no data were presented to support this conclusion. It was not possible to propose a NOAEL for maternal toxicity. The NOAEL for developmental toxicity is, however, considered to be greater than the highest dose tested, 1,000 mg/kg bw/day. A LOAEL for maternal toxicity is 100 mg/kg bw, based on the increased liver weights.	Brooke et al. 2009 (study presented in Akzo Nobel, 2004 as well).	Reported in a secondary source (review)
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	No data located		
	Prenatal Development	No data located		
	Postnatal Development	No data located		
	Prenatal and Postnatal Development	No data located		

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Property/Endpoint		**Data**	**Reference**	**Comments**
	Developmental Neurotoxicity	No data located		
	Other	No data located		
Neurotoxicity (single dose and repeated)		**MODERATE:** Based on significant inhibition (56%) of plasma cholinesterase activity, but no inhibition of NTE activity after repeated dosing. Phosflex 5 1B caused cholinesterase inhibition at a single very high dose of 10 ml/kg (11.7 g/kg), but no evidence of cholinesterase inhibition at significantly lower doses. There is potential for neurotoxic effects based on a structural alert for organophosphates .		
	Acute and delayed neurotoxicity tests in hens	Test substance was the commercial product Phosflex 51B. 15 adult hens, exposed to 11.7 g/kg at the start of the study and again 21 days later, and all hens were terminated 21 days after the second dose. A negative and a positive control was included in the study as well. Phosflex 5 1B administered to hens at the very high dose of 11.7 g/kg did not cause neurotoxicity.	Akzo Nobel, 2004	Reported in a secondary source.
		Test substance was the commercial product Phosflex 51B. 4 adult hens/group, 3 groups in total received a single oral gavage dose of 10 ml/kg. A positive control (TOCP) was also included. The animals were terminated after 24 h, and plasma cholinesterase activity and brain neurotoxic esterase (NTE) activity were measured. Phosflex 5 1B produced significant inhibition (56%) of plasma cholinesterase activity, but did no inhibit NTE activity (0% inhibition). Although Phosflex 5 1B caused cholinesterase inhibition at the very high dose of 10 ml/kg (11.7 g/kg), there is no evidence that the substance causes cholinesterase inhibition at significantly lower doses, which would be more representative of levels of human exposure. The authors concluded that Phosflex 5 1B did not demonstrate neurotoxic activity.	Akzo Nobel, 2004	Reported in a secondary source. EPA OTS Guideline for Acute Neurotoxicity Testing, no GLP
		Test substance was the commercial product Durad 220B. 3 groups of adults hens (9 per group) received a single oral dose of either Durad (2 g/kg), tap water, or a positive control. Brain and spinal cord neurotoxic esterase (NTE) activity and brain acetylcholinesterase activity was measured in 3 hens per group 48 hours after dosing. The remaining hens were	Akzo Nobel, 2004	Reported in a secondary source. EPA OTS Guideline for Acute Neurotoxicity Testing, no GLP

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Property/Endpoint		**Data**	**Reference**	**Comments**
		sacrificed after 21 days observational period. No inhibition of brain or spinal cord NTE activity or brain acetylcholinesterase activity was observed in Durad 220B treated hens, and Durad 220B did not express neurotoxic activity.		
		The neurotoxic potential of a jet engine lubricant containing synthetic turbo jet oil and 3 % butylated triphenyl phosphate (100% mixture of butyl and triphenyl phosphate mixtures). Groups of 17-hens were given the test substance by oral gavage at a limit dose of 1 g/kg, 5 days a week for 13 weeks. A positive and negative control was also included. NTE and AChE activities were assayed in 2brain and spinal cord from 4 hens in each group after 6 and 13 weeks of dosing. NTE and AChE activity was not significantly different from control after 6 weeks dosing, but NTE actively was inhibited 23-34% in brains of lubricant treated hens. AChE activity was not inhibited after either 6 or 13 weeks. There was no difference in the clinical assessments between the lubricant treated hens and the negative control group. There was no indication of organophosphorus-induced delayed neuropathy (OPIDN).	Daughtrey et al. 1996, Brooke et al. 2009	Primary source. Also reported in a secondary source.
	Other	There is potential for neurotoxic effects based on a structural alert for organophosphates (Estimated)	Expert judgement	Estimated based on a structural alert for organophosphates.
Repeated Dose Effects		**MODERATE:** Based on the liver and kidney weight effects observed at the highest orally administered dose in a 90-day study and a NOEL of 26.7 mg/kg bw/day, and a dermal NOAEL of 10 mg/kg bw/day based on evident dose response depression of terminal cholinesterase.		
	Sub-chronic oral repeated dose	90 days repeated dose oral exposure study in rats. Exposed to the commercial product Phosflex 51B blended in the diet at doses of 0, 100,400, or 1600 ppm. Parameters measured include body weight, food consumption, clinical observations, hematology, clinical chemistry, and cholinesterase activity. Based on the organ weight effects (liver and kidney) observed	Akzo Nobel, 2004; Brooke et al. 2009. Primary source: Freudenthal et al. 2001	Reported in a secondary source – consistent with data in the primary source.

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Property/Endpoint		**Data**	**Reference**	**Comments**
		at the highest dose of Phosflex 51B, the NOEL for this study is 26.7 mg/kg bw/day in male rats or 30.0 mg/kg bw/day in female rats (equivalent to 400 ppm).		
		Phosflex 51B was administered to rats in concentrations of 0, 100, 400 and 1600 ppm by diet (= mg/kg food) was not regarded as a toxic and therefore not an adverse effect. Under the conditions of this study, the 90-day administration of Phosflex 51B by diet in rats showed to induce no adverse effects. Therefore, a NOAEL of 107.5 and 124.8 mg/kg bw/day (equivalent to 1600 ppm) was established for males and females, respectively.	REACH registration data	Reported in a secondary source. Same study as reported above, however different conclusion regarding the NOAEL value. Not consistent with the primary source (Freudenthal et al. 2001).
	Sub-chronic inhalation repeated dose	The toxicity of the commercial product Santicizer 154 was determined in a 90-day inhalation study in rats. Male and female animals were exposed for 6 hours a day, 5 days a week to 0, 10.1 or 101.1 mg/m³. Under the conditions of the study, no clear test article- or dose-related effects were observed in rats as a result of exposure to Santicizer 154. Therefore, a NOAEL of 101.1 mg/m³ was established.	REACH registration data	Reported in a secondary source. Study was conducted according to a method comparable to OECD guideline 413, but not under GLP conditions. Reliability 2.
	Dermal repeated dose	The toxicity of the commercial product Santisizer 154 was determined in a 21-day repeated dose dermal toxicity study in rabbits. Santicizer-154, at dose levels of 10, 100 and 1000 mg/kg/day, was applied to the clipped dorsal surface of New Zealand White rabbits daily, 5 days per week for three weeks. Based on evident dose response depression of terminal cholinesterase in the Santicizer-154 treated males and females, which was significant in the mid and high dose, a NOAEL of 10 mg/kg bw/day was derived	REACH registration data	Reported in a secondary source. Study was not conducted under GLP, but was performed according to methods similar to OECD guideline 410. Reliability 2.
Skin Sensitization		**LOW:** Expert judgement based on human patch testing of 50 subjects with no sensitisation supported by human evidence from occupational use. No classification suggested.		
	Skin sensitization	The commercial product Phosflex 71B did not indicate a potential for dermal irritation or allergic contact sensitiza-	REACH registration data	Reported in a secondary source. Non-international guideline, GCP compliance.

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Property/Endpoint		**Data**	**Reference**	**Comments**
		tion.		Reliability 1.
	Skin sensitization in humans	Based on 2 years of experience with the substance in various products on the production facility in Gallipolis Ferry, WV, US, there have been no incidences of sensitization of workers known to the management related to the use and production of the substance Phenol, isobutylated, phosphate (3:1) at the GF facility in the US. (data from workplace)	REACH registration data	Reported in a secondary source. Reliability 1.
Respiratory Sensitization		**No data.**		
	Respiratory Sensitization	No data located		
Eye Irritation		**MODERATE:** Fully reversible effects within 48 hours.		
	Eye Irritation	Mild redness of the conjunctiva was observed in two rabbits (one with a washed eye, the other with an unwashed eye) at the 24 hour observation. The two eyes cleared by 48 hours, but another eye (unwashed) showed mild redness of the conjunctiva at 48 hours. All eyes were clear of irritation at 72 hours and 96 hours, and remained so through the 7 day observation. The average irritation scores at 24 and 48 hours were 0.44 and 0.22, respectively, thus Phosflex 5 1 B is a very mild eye irritant.	Akzo Nobel, 2004, Brooke et al. 2009	Reported in a secondary source. Guideline EPA OTS 798.4500, no GLP compliance. Reliability 1 according to Akzo Nobel.
		The commercial product Phosflex 72B was a non-irritant in the eyes of albino rabbits. This formulation produced no eye irritation in rabbits whose eyes were left unwashed or in rabbits whose eyes were washed 20-30 seconds after treatment.	REACH registration data	Reported in a secondary source. Non-GLP study according to EPA Guideline, which is consistent with OECD Guideline 405, 1981. Reliability 2
Dermal Irritation		**MODERATE:** Fully reversible effects within 72 hours.		
	Dermal Irritation	Mild to moderate erythema was observed 24 hours after treatment; the number of rabbits with erythema was not reported. At 48 hours after treatment, mild erythema was	Akzo Nobel, 2004, Brooke et al. 2009	Reported in a secondary source. Guideline EPA OTS 798.4470, no GLP compliance. Reliability 1 according to Akzo Nobel.

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Property/Endpoint		**Data**	**Reference**	**Comments**
		present in four of the individual animals, but at 72 hours no irritation was present. No observations of oedema were made. Primary irritation score was 0.5, indicating that the commercial product Phosflex 51B is a mild skin irritant.		
		The commercial product Phosflex 72B produced mild erythema (4 rabbits) and mild oedema (1 rabbit) in intact and abraded skin of albino rabbits following a 24 hour exposure. At the 72 hour observation, irritation decreased and included mild erythema in one of the six rabbits (no 14 days observation period done for reversibility). Primary irritant score was 0.46	REACH registration data	Reported in a secondary source. Non-GLP study according to EPA Guideline. Reliability 2
Endocrine Activity		**No data**		
	Endocrine activity	No data located		
Immunotoxicity		**No data**		
	Immune System Effects	No data located		

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0			
Property/Endpoint	**Data**	**Reference**	**Comments**
Ecotoxicity			
ECOSAR Class	Esters, esters (phosphate)		
Aquatic Acute Toxicity	**VERY HIGH:** Based on experimental EC_{50}'s for daphnia ranging from 0.2 – 0,289 mg/L. Also one fish LC_{50} is below 1 mg/L.		
Fish LC_{50} (Freshwater)	LC_{50} 96h: 0.8 mg/L (0.6 – 1.0 mg/l) (*Ictalurus punctatus*) (experimental) (test substance was the commercial product Fyrquel GT)	REACH registration data; Brooke et al. 2009	Reported in a secondary source.
	LC_{50} 96h : 13.7 mg/L (*Salmo gairdneri*) (experimental) (test substance was the commercial product Fyrquel GT)	Akzo Nobel, 2004	Reported in a secondary source, guideline study, but no GLP
Fish LC_{50} (Marine)	LC_{50} 96h: >1 mg/L (*Cyprinodin variegatus*) (experimental) (test substance tert-butylphenyl diphenyl phosphate)	Akzo Nobel, 2004	Reported in a secondary source, guideline study with GLP
Daphnid LC_{50} / EC_{50} (Freshwater)	EC_{50} 48h: 0.25 – 5 mg/L (*Daphnia magna*) (experimental, range from several studies) (test substance tert-butylphenyl diphenyl phosphate)	Brooke et al. 2009	Reported in a secondary source.
	EC_{50} 48h: 0.2-0.289 mg/L (*Daphnia magna*) (experimental) (test substance commercial product Santicizer 154)	REACH registration data	Reported in a secondary source
Daphnid LC_{50} / EC_{50} (Marine)	EC_{50} 96h: 0.39 mg/L (*Mysidopsis bahia*) (experimental) (test substance tert-butylphenyl diphenyl phosphate)	Akzo Nobel, 2004	Reported in a secondary source, guideline study with GLP
Green Algae IC_{50} / EC_{50}	EC_{50} 96h: 2.6 ppm (2.6 mg/L). Endpoint: decrease in cell no. (*Selenastrum capricornutum*) (experimental) (test substance Santicizer 154)	Akzo Nobel, 2004	Reported in a secondary source, guideline study but no GLP. Also referred to in Brooke et al., 2009, where the study is assessed as not assignable.
Aquatic Chronic Toxicity	**VERY HIGH:** Based on experimental chronic (21d) NOEC's for daphnia ranging from 0.01 to 0,.04 mg/L		
Fish ChV NOEC (Freshwater)	NOEC 90 d: 0.194 mg/L (growth) 0.093 mg/L (mortality) (*Pimephales promelas*) (experimental) ((test substance was the commercial product Fyrquel	REACH registration data, Brooke et al. 2009	Reported in a secondary source.

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Property/Endpoint		**Data**	**Reference**	**Comments**
		GT)		
Daphnid NOEC (Freshwater)		NOEC 21 d: 0.01-0.04 mg/L (*Daphnia magna*) (experimental) (test substance tertbutylphenyl diphenyl phosphate)	Brooke et al. 2009	Reported in a secondary source.
		NOEC 21d: 0.040 mg/l (*Daphnia magna*) (experimental) (test substance commercial product Santicizer 154)	Akzo Nobel, 2004	Reported in a secondary source.
Green Algae NOEC		NOEC 14d: 1.0 mg/L (*Selenastrum capricornutum*) (experimental)	Brooke et al. 2009	Reported in a secondary source. Assessed by authors as not valid study.
Transport		Results of Level III fugacity modelling indicate that at equilibrium the substance will be found almost exclusively in water (55%) and sediment (45%). The expected mobility in soil is moderate based on an estimated K_{OC} of about 4,800. The vapour pressure of the substance is low and the Henry's Law Constant indicates that the volatility from water surfaces will also be low (approx.. same rate as water) and in the atmosphere the substance is therefore expected to be present mainly associated with water aerosols and removal from air therefore primarily by wet deposition.		
	Henry's Law Constant (atm-m^3/mole)	0.009 Pa m^3/mole at 20°C (for tert-butylphenyl diphenyl phosphate) (estimated based on compound structure)	Brooke et al. 2009	Reported in a secondary source (review)
		8.9 × 10-7 atm-m^3/mole (estimated)	US EPA 2008	Reported in a secondary source.
	Sediment/Soil Adsorption/Desorption – K_d/K_{oc}	Koc = 4,773 L/kg (tert-butylphenyl diphenyl phosphate) (estimated based on compound log Kow)	Brooke et al. 2009	Reported in a secondary source (review)
	Level III Fugacity Model	Air 2.5 × 10^{-3} % Water 54.9 % Soil 7.5 × 10^{-3} % Sediment 45.1 % (estimated)	US EPA 2008	Reported in a secondary source.
		Air 0.27 % Water 10 % Soil 79.4 % Sediment 10.4% (estimated)	Brooke et al. 2009	Reported in a secondary source (review). Based on emission of 1000 kg/hour to soil, water and air, respectively.

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Property/Endpoint		**Data**	**Reference**	**Comments**
Persistence		**LOW:** The substance was found to be readily biodegradable in an OECD screening test (measured). There is no data for the possible biodegradation in soil but in water/sediment system studies primary degradation was found to be rapid with half-lives from <0.5 days to 3 days. In one study 1.7% to 37% full mineralisation was found to take place within 8 weeks, depending on test substance concentration. Atmospheric half-life estimated to be 24 hours. Results of experimental studies of abiotic degradation by photolysis or hydrolysis indicate that these processes are likely to be of low importance in the environment.		
Water	Aerobic Biodegradation	Readily biodegradable: Degraded 61% after 28 days in closed bottle test (OECD 301D). Test parameter: O_2 consumption. It is stated that the test validity criteria were met, but no mentioning of 10-day (or 14-day) window fulfilment (measured)	REACH registration data	Reported in a secondary source, (standardised test method)
	Volatilization Half-life for Model River	No data located		
	Volatilization Half-life for Model Lake	No data located		
Soil	Aerobic Biodegradation	No data located		
	Anaerobic Biodegradation	No data located		
	Soil Biodegradation with Product Identification	No data located		
	Sediment/Water Biodegradation	Half-life: < 0.5 for triphenyl phosphate 1 day for t-butylphenyldiphenyl phosphate 7 days for di(t-butylphenyl) phenyl phosphate (Test substance was the commercial product Santicizer(r) 154) (measured)	REACH registration data	Reported in a secondary source. Study carried out according to well described method and with GLP, but not according to international guideline

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Property/Endpoint		**Data**	**Reference**	**Comments**
		Half-life for primary degradation: 1-3 days for a mixture of triphenyl phosphate and tributylphenyl diphenyl phosphate in microcosm test with lake water and sediment. 2-3 days for a mixture of triphenyl phosphate and tributylphenyl diphenyl phosphate in outdoor simulation test with well water and river sediment. (measured)	Brooke et al. 2009	Reported in a secondary source (review).
		"Experiments investigating degradation in sediments have generally shown reasonably rapid primary degradation (half-lives of 1 to 3 days in some experiments have been seen), but one series of experiments using sediment microcosms found that the rate of mineralisation depended on the actual concentration of the test substance; mineralisation rates of 1.7 per cent up to 37 per cent over eight weeks were seen in these studies. The default mineralisation half-life of 90 days estimated above appears to be consistent with these data." (estimated based on identified data data)	Brooke et al. 2009	Expert judgement based on available data
Other	Biotic degradation.	28 fungi capable of metabolising tert-butylphenyl diphenyl phosphate have been identified. The main products formed were alkyl side chain-oxidised and aromatic ring-oxidised metabolites, with di- and monoaryl phosphates formed to a lesser extent.	Brooke et al. 2009	Reported in a secondary source (review).
Air	Atmospheric Half-life	24 h (for tert-butyl phenyl diphenyl phosphate) (estimated on basis of the compound structure)	Brooke et al. 2009	Reported in a secondary source (review).
Reactivity	Photolysis	Half-life > 14 days (test substance commercial product Santicizer(r) 154 (measured)	Akzo Nobel, 2004	Reported in a secondary source.
		Half-life infinite (tert-butylphenyl diphenyl phosphate) (estimated based on measured data	Brooke et al. 2009	Reported in a secondary source (review). Estimate is based on collaboration of

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0				
Property/Endpoint		**Data**	**Reference**	**Comments**
				available information as well as expert judgement by the authors.
		Half-life >28 h (for the commercial product Santicizer(r) 154 (tert-butylphenyl diphenyl phosphate) (measured)	REACH registration data	Reported in a secondary source.
	Hydrolysis	Half-life at 25°C: 60 days at pH 4; 14 days at pH 7; 5.4 days at pH 9 At 15°C: >100 days at pH 4; 28 days at pH 7; 15 days at pH 9 (test substance butylated triphenyl phosphate) (measured)	Akzo Nobel, 2004	Reported in a secondary source.
		Half-life infinite (tert-butylphenyl diphenyl phosphate) (estimated based on measured data	Brooke et al. 2009	Reported in a secondary source (review). Estimate is based on collaboration of available information as well as expert judgement by the authors.

Phenol, isobutylenated, phosphate/CAS No. 68937-40-6/EC No. 273-065-8/700-990-0				
Property/Endpoint		**Data**	**Reference**	**Comments**
Environmental Half-life		No data located		
Bioaccumulation		**MODERATE:** Based on measured BCFs for fish in the range 778-1850 and an estimated BCF for earthworms of 1583. Log Kow values are in the range 4.8 to 6.6 thus indicating an even higher bioaccumulation potential. However, measured BCF values have preference over predictions based on Kow.		
	Fish BCF	778 L/kg (for ^{14}C-labelled tert-butylphenyl diphenyl Phosphate) (estimated based on identified BCF data)	Brooke et al. 2009	Reported in a secondary source (review). Estimate is based on collaboration of available information as well as expert judgement by the authors.
		1850 for t-butylphenyldiphenyl phosphate (Test substance was the commercial product Santicizer(r) 154) (calculated based on measured data)	REACH registration data	Reported in a secondary source.
	Other BCF	BCF for earthworms: 1,583 L/kg (estimated based on the log Kow)	Brooke et al. 2009	Reported in a secondary source (review). Authors report that the reliability of the estimate is unknown.
	BAF	No data located		
	Metabolism in Fish	No data located		
Environmental biomonitoring				
Ecological Biomonitoring		No data located		
Human Biomonitoring		No data located		

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REACH registration data: http://echa.europa.eu/da/information-on-chemicals/registered-substances using CAS No. 68937-40-6 as search term.

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Appendix 6 Phosphinic acid, aluminium salt (3:1), CAS No. 7784-22-7

No harmonized classification (CLP) is available for the substance. 356 of 364 industry notifications suggest a classification with Aquatic Chronic 3 (as of 11.10.2015).
Apart from REACH registration data, no other data sources provide information on the substance. QSAR estimations are not appropriate because the substance is inorganic.

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8			
Property/Endpoint	**Data**	**Reference**	**Comments**
Physical/chemical properties			
Melting Point (°C)	≥ 310 °C Decomposition occurs before melting.	REACH registration data	Reliability 1 Study conducted according to internationally accepted testing guidelines and performed according to GLP.
Boiling Point (°C)	Data waiving	REACH registration data	
Vapour Pressure (Pa)	Data waiving	REACH registration data	
Water Solubility (mg/L)	ca. 24000 mg/L at 20 °C, pH ca. 3.2	REACH registration data	Reliability 1 GLP compliant with international guideline
Log Kow	Data waiving	REACH registration data	Inorganic substance
pKa	No data located.		

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
Human health effects				
Toxicokinetics				
Dermal absorption *in vitro*		No data located.		
Absorption, Distribution, Metabolism & Excretion	Oral and intravenous	Absorption and distribution of aluminium following and intravenous + oral administration of Sprague-Dawley rats at a dose equivalent to 8.1 mg/kg one per day, two days exposure. Main ADME results: *absorption* 27% from oral *distribution* plasma *metabolism* none *excretion* 27% urine, remaining faeces as not absorbed	REACH registration data	Reliability 2 Old study (1986) plus Reviews from authorative source
Acute mammalian toxicity		**LOW:** Based on the oral LD50 in rats of >2,000 mg/kg and the dermal LD50 in rabbits of >2,000 mg/kg. The study on inhalation exposure was evaluated to be insufficient for consideration for the score.		
Acute lethality	Oral	Six Sprague-Dawley rats were exposed to 2000 mg/kg bw. LD50 > 2000 mg/kg bw	REACH registration data	Reliability 2 Study conducted according to OECD Guideline 423 and performed according to GLP. Nevertheless, many details were missing and no information about the test material is available.
	Dermal	5 female and 5 male Sprague-Dawley were exposed for 24 hr to 2000 mg/kg bw. LD50 > 2000 mg/kg bw	REACH registration data	Reliability 1 Study conducted according to OECD Guideline 402 and performed according to GLP.
	Inhalation	5 male and 5 female Wistar rats were exposed to 3.30 mg/l for 4 hours. Nose only the snouts and nostrils of the animals	REACH registration data	Reliability 1 Study conducted according to OECD

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
		were exposed to the aerosol. LC50 (4h) > 3.30 mg/l (only dose tested) Considering the fact that no mortality occurred, a classification category cannot be assigned.		Guideline 403 and performed according to GLP.
Carcinogenicity		**DG**		
	QSAR results from the literature (e.g. Danish QSAR database)	Not applicable.		
	Carcinogenicity (Rat and Mouse)	No data located.		
	Combined Chronic Toxicity/Carcinogenicity	No data located.		
Genotoxicity		**LOW:** Negative in *in vitro* Mammalian chromosome aberration test and *in vivo* micronucleus assay.		
	Gene Mutation *in vitro*	No data located.		
	Gene Mutation *in vivo*	No data located.		
	Chromosomal Aberrations *in vitro*	Mammalian chromosome aberration test Concentration range in the main test (with metabolic activation): 45, ..., 405 µg/ml Concentration range in the main test (without metabolic activation): 38, ..., 650 µg/ml Exposure period (with metabolic activation): 3 hours Exposure period (without metabolic activation): 21 hours. There was no evidence of induction of chromosome aberrations either in the presence or absence of metabolic activation,	REACH registration data	Reliability 1 OECD Guideline 473
	Chromosomal Aberrations *in vivo*	Micronucleus assay with mouse exposed via two oral gavages (two treatments at 24 hour intervals) to 0, 250, 500 and 1000 mg/kg bw. Aluminium hypophosphite was concluded to be negative in	REACH registration data	Reliability 1 GLP compliant with international (OECD Guideline 474) and Asian guideline

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
		the *in vivo* mouse micronucleus assay.		
	DNA Damage and Repair	No data located.		
Reproductive effects		**LOW:** NOAEL > 1000 ppm in a reproduction/developmental toxicity Screening study.		
	Reproduction/Developmental Toxicity Screen	Male and female Wistar rats were exposed to 0, 100, 300, 1000 ppm nominal in the diet for 2 consecutive weeks prior to pairing and thereafter during pairing, post coitum and post partum periods until Day 4. NOAEL (general toxicity and for fertility and reproduction parameters) male was considered to be the highest dose tested, i.e. 1000 ppm (corresponding to 77 mg/kg bw/day; actual dose received) NOAEL (general toxicity and for fertility and reproduction parameters) female was considered to be the highest dose tested, i.e. 1000 ppm (corresponding to 95 mg/kg bw/day (actual dose received)	REACH registration data	Reliability 1 Study conducted according to OECD Guideline 421 and 422 and performed according to GLP.
	Continuous breeding study	No data located.		
	Combined Repeated Dose with Reproduction/Developmental Toxicity Screen	No data located.		
	Reproduction and Fertility Effects	No data located.		
Developmental effects		**LOW:** NOAEL > 1000 ppm in a reproduction/developmental toxicity Screening study.		
	Reproduction/Developmental Toxicity Screen	Males were treated for 2 weeks prior to pairing and during pairing with females until the day before necropsy, for a total of 29 days. Females were treated for 2 weeks prior to pairing, during	REACH registration data	Reliability 1 Study conducted according to OECD Guideline 421 and performed according to GLP.

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
		pairing and throughout the gestation and lactation periods until Day 3 post partum. Pups: until Day 4 post partum. Doses of 0, 100, 300, 1000 ppm nominal in the diet. No treatment-related effects were observed for these parameters. Litter data and sex ratios were unaffected by treatment. Clinical signs of pups: There were no treatment-related effects. Necropsy findings in decedent pups and in pups sacrificed on Day 4 post partum did not reveal any treatment-related effect. NOAEL for general toxicity and for fertility and reproduction parameters was considered to be the highest dose tested, i.e. 1000 ppm for males and females (corresponding to 77 and 95 mg/kg bw, respectively).		
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	No data located.		
	Prenatal Development	No data located.		
	Postnatal Development	No data located.		
	Prenatal and Postnatal Development	No data located.		
	Developmental Neurotoxicity	No data located.		
Neurotoxicity				
	Acute and delayed neurotoxicity tests in hens	No data located.		

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
Repeated Dose Effects		**Moderate:** Based on the NOAEL of ca. 35.2 mg/kg bw/day. There is uncertainty about repeated dose effects, because no concentrations with significant toxic effects were reported and no 90-day exposure study is available. The score is based on a conservative approach.		
	Sub-chronic oral repeated dose	Phoslite IP-A was administered to Wistar rats (5 animals/sex/group) in the diet for 4 weeks at doses of 0, 100, 300, 1000 ppm, equal to compound intake of 0, 9.9, 27.8 and 86.9 mg/Kg/bw on males and 0, 11.4, 35.2 and 121.2 mg/Kg/bw on females. NOAEL female rats: ca. 35.2 mg/kg bw/day (nominal) NOAEL male rats: ca. > 86.9 mg/kg bw/day (nominal) Effects based on increased platelet count and mean corpuscular haemoglobin concentration and a decrease of haematocrit.	REACH registration data	Reliability 1 Full GLP study, OECD guideline 407
	Sub-chronic inhalation repeated dose	Data waiving	REACH registration data	
	Dermal repeated dose	Data waiving	REACH registration data	
Skin Sensitization		**LOW:** Negative		
	Skin sensitization	Female guinea pig, intradermal induction and challenge exposure to test item at 50% concentration in sterile water. Conclusion: not sensitising	REACH registration data	Reliability 1 OECD guideline 406
	Skin sensitization in humans	No data located.		
Respiratory Sensitization		**DG**		
	Respiratory Sensitization	No data located.		
Eye Irritation		**MODERATE:** Fully reversible effects within 7 days.		
	Eye Irritation	3 New Zealand White rabbits were exposed for 7 days to 100 mg of the test item.	REACH registration data	Reliability 1 OECD guideline 405

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
		Observation after 1, 24, 48, 72 hours and 7 days. 1-hour after application the following ocular reactions were observed: iritis grade 1 in 1/3 test eyes; redness grade 2 in 2/3 test eyes and grade 1 in 1/3 test eyes; chemosis grade 2 in 1/3 test eyes and grade 1 in 2/3 test eyes. Reversibility of any observed effect: Changes fully reversible within 7 days. Conclusion: not irritating		
Dermal Irritation		**LOW:** No irritation was observed.		
	Dermal Irritation	3 New Zealand White rabbits were exposed for 4 hr to 500 mg of the test item. No irritation was observed. Conclusion: not irritating	REACH registration data	Reliability 1 OECD guideline 404
Endocrine Activity		**DG**		
	Endocrine activity	No data located.		
Immunotoxicity		DG		
	Immune System Effects	No data located.		

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8			
Property/Endpoint	**Data**	**Reference**	**Comments**
Ecotoxicity			
ECOSAR Class	None (Inorganic compound)		
Aquatic Acute Toxicity	**Moderate:** Based on a EC50 (biomass) of ca. 29 mg/L in an algae growth inhibition test with *Pseudokirchneriella subcapitata*		
Fish LC_{50} (Freshwater)	Static test with *Danio rerio* exposed to a nominal concentration of 100 mg/L 96 h, LC50 > 100 mg/L	REACH registration data	Reliability 2 According to OECD Guideline 203. The concentration of the substance tested was not satisfactorily maintained throughout the test
Fish LC_{50} (Marine)	No data		
Daphnid LC_{50} / EC_{50} (Freshwater)	Static *Daphnia* sp. Acute Immobilisation Test, exposure to a nominal concentration of 100 mg/L. 48 h, EC50 (immobilisation) > 100 mg/L	REACH registration data	Reliability 2 Study conducted according to OECD Guideline 202 and performed according to GLP. The average analytical recovery of phosphorus (P) was 87.6 % during the exposure period, while the analytical recovery of aluminium (Al) was lower than the Limit Of Detection of the analytical method (LOD: 0.25 mg AI/l) already immediately after the test solution preparation. These results were likely due to the precipitation of aluminium in the test medium.
Daphnid LC_{50} / EC_{50} (Marine)	No data		

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8			
Property/Endpoint	**Data**	**Reference**	**Comments**
Green Algae IC_{50} / EC_{50}	Growth Inhibition Test with *Pseudokirchneriella subcapitata* with nominal concentrations of 10.0 ,17.8 , 31.6, 56.2 and 100 mg/L. 72 h, EC50 (growth rate) > 100 mg/L 72 h, EC50 (biomass) ca. 29 mg/L	REACH registration data	Reliability 2 Study conducted according to OECD Guideline 201 and performed according to GLP.
Microorganisms IC_{50} / EC_{50}	Static test with domestic, activated sludge at nominal concentrations of 1.0, 3.2, 31.6 and 100 mg/L, exposure duration 3 hr. 3 h, IC50 (respiration rate) > 100 mg/L 3 h, NOEC (respiration rate) 31.6 mg/L	REACH registration data	Reliability 1 Study conducted according to OECD Guideline 201 and performed according to GLP.
Aquatic Chronic Toxicity	**Moderate:** Based on notified classification, because experimental data are insufficient.		
Fish NOEC (Freshwater)	Semi-static test with *Danio rerio* exposed for 14 days to nominal concentrations of 4.48, 9.86, 21.7, 47.7 and 105 mg/L 14 d, NOEC (mortality) 105 mg/L The study is a prolonged toxicity test and thus not sufficient for assessing chronic toxicity.	REACH registration data	Reliability 2 Study conducted according to OECD Guideline 204 and performed according to GLP. The substance concentration has not been satisfactorily maintained throughout the test: the elemental analytical concentrations were in the range 90 - 103 % in the case of phosphorus, but they were in the range of 0.20 – 22.30 % in the case of the aluminium.
Daphnid NOEC (Freshwater)	No data		
Green Algae NOEC	No data		
	Aquatic Chronic 3, H412	C&L Inventory	Notified classification and labelling
Transport	The substance is an inorganic salt, which according to information from the registrant is fully soluble and fully dissociated in its ionic forms (at the concentrations tested in the adsorption study). Phosphorus was fully recovered (80~120 %), indicating that the phosphorus-containing component (phosphinic acid) does not adsorb in soil. The study does not provide any details on aluminium adsorption. In the		

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
		atmosphere, the substance is expected to be present only associated with water aerosols and removal from air is therefore by wet deposition. The substance will therefore be found almost exclusively in the water compartment.		
	Henry's Law Constant (atm-m^3/mole)	No data		
	Sediment/Soil Adsorption/Desorption – K_d/K_{oc}	The analysis of Phoslite IP-A is conducted with HPLC for determination in soil and water. The method was developed to determine the total phosphorus in water and soil using the ammonium molybdate spectrophotometric method (λ = 700 nm with Agilent Vis-UV 8453), to calculate the Phoslite IP-A content through the determination of phosphorus in this environment. Adsorption of Phoslite IP-A was tested in triplicate on three different soils: Black, Brown and Red at concentrations of 48.0, 72.0 and 96.0 µg/ml. Results show the method is fit for determination of Phoslite IP-A in soil and that the recovery of Phoslite IP-A in chernozem, brown soil, red soil and cinnamon soil is range from 80~120 %. Conclusion of the study: Phoslite IP-A is an inorganic salt, which is fully soluble and fully dissociated in its ionic forms. As expected, there is no adsorption in soil.	REACH registration data	Reliability 2 Study conducted according to internationally accepted testing guidelines and performed according to GLP. Nevertheless, only non-official English translation is available.
	Level III Fugacity Model	Not applicable		
Persistence		**Very high**: Phosphinic acid is not expected to be degraded by hydrolysis and the metal ion is recalcitrant. Information about other environmental degradation pathways for phosphinic acid are lacking.		
Water	Aerobic Biodegradation	Data waiving		

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Volatilization Half-life for Model River	No data		
	Volatilization Half-life for Model Lake	No data		
Soil	Aerobic Biodegradation	Data waiving	REACH registration data	
	Anaerobic Biodegradation	No data		
	Soil Biodegradation with Product Identification	No data		
	Sediment/Water Biodegradation	No data		
Other	Biotic degradation.	No data		
Air	Atmospheric Half-life	No data		
Reactivity	Photolysis	No data		
	Hydrolysis	Read-across with sodium phosphinate (structural analogue or surrogate) In the test conditions, the tests at pH 4.0, pH 7.0 and pH 9.0 showed no significant degradation of sodium phosphinate (Solid) at 50 °C. The hydrolysis of sodium phosphinate (Solid) was less than 10% after 5 days. As no degradation was observed, sterility tests were not considered as needed. Therefore, the estimated half-life time is higher than one year under representative environmental conditions (25 °C). Therefore, sodium phosphinate (Solid) and phosphinic acid are considered to be hydrolytically stable.	Reach registration data for phosponic acid (CAS nr. 6303-21-5)	Reliability 2 (reliable with restrictions), according to OECD Guideline 111 (Hydrolysis as a Function of pH)

Phosphinic acid, aluminium salt (3:1) /CAS No. 7784-22-7 /EC No. 479-150-8				
Property/Endpoint		**Data**	**Reference**	**Comments**
Environmental Half-life		No data		
Bioaccumulation		**LOW:** The substance is not expected to have potential for bioaccumulation based on professional judgement.		
	Fish BCF	No data		
	Other BCF	aquatic / sediment Data waiving	REACH registration data	
	BAF	No data		
	Metabolism in Fish	No data		
Environmental biomonitoring				
Ecological Biomonitoring		No data		
Human Biomonitoring		No data		

C&L Inventory: http://echa.europa.eu/information-on-chemicals/cl-inventory-database using CAS No. 7784-22-7 as search term.

REACH registration data: http://echa.europa.eu/da/information-on-chemicals/registered-substances using CAS No. 7784-22-7 as search term.

Appendix 7 Melamine phosphate (1,3,5-triazine-2,4,6-triamine phosphate), CAS No. 41583-09-9

This profile is for melamine phosphate (1,3,5-triazine-2,4,6-triamine phosphate, CAS No. 41583-09-9). Only few data are available. Most data in the REACH registration dossier are based on the substance melamine. The substance does not have a harmonised CLP classification. All notifiers, except one, suggest "no classification".

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7			
Property/Endpoint	**Data**	**Reference**	**Comments**
Physical/chemical properties			
Melting Point (°C)	The substance decomposes before melting. Decomposition temperature of 350°C, no sublimation	REACH registration data	Reliability 2 non GLP, non-standard method (Thermogravimetric analysis), no details on test item, but method well described.
Boiling Point (°C)	Data waiving	REACH registration data	
Vapour Pressure (Pa)	Data waiving	REACH registration data	
Water Solubility (mg/L)	3900 mg/L at 20°C	REACH registration data	Reliability 1 (standardised guidelines)
	max. 5 g/l (for the commercial product MPT11)	Metadynea, 2014	
	<3 g/l (for the commercial product Melapur® MP)	BASF, 2010	
Log Kow	- 3.0	REACH registration data	Reliability 2 (OECD 107 + GLP compliant, but water solubility not checked for the estimation method)
pKa	Read-across based on grouping of substances. The pKa values are 5.39, 3.05 and 0.48.		Reliability 2 Scientifically acceptable software
	Read-across based on grouping of substances. The pKa values are 2.21, 7.21 and 12.38.		Reliability 2 Authoritative handbook
	Read-across based on grouping of substances. The pKa is 5.		Reliability 2 Peer reviewed database
	Read-across based on grouping of substances.		Reliability 2

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7			
Property/Endpoint	**Data**	**Reference**	**Comments**
	The pKa values are 2.15, 7.09 and 12.32.		Authoritative handbook
Other relevant physical/chemical properties	The test substance is not considered highly flammable.		

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
Human health effects				
Toxicokinetics				
Dermal absorption *in vitro*		No data located		
Absorption, Distribution, Metabolism & Excretion	Oral	Metabolism, disposition and excretion of 14C-Melamine (CAS No. 108-78-1) in male Fischer 344 rats after administration of a single oral dose of 0 .025 mCi/rat (approximately 1 .3 mg/kg body weight). Distribution: Concentrations of [14C]melamine in the blood, plasma, bladder, liver, kidney and ureter of male Fischer 344 rats treated orally with a single dose were generally very low (0 – 12 pbb). Excretion: The percentages of radioactivity present as melamine in the urine, blood, plasma and faeces after 0.5, 1.0, 4.0, 8.0, 24.0, 48.0, 72.0, and 96.0 were generally high (ranging between 94.9 and 99.5% of total). Conclusion: No bioaccumulation potential based on study results	REACH registration data	Reliability 2 Comparable to guideline study with acceptable restrictions (only one dose level tested), read-across from supporting substance (structural analogue or surrogate)
	Oral	Clinical test in man. Melamine is a metabolite of hexamethylmelamine after demethylation steps. The experiments indicate that the s-triazine ring is very stable and that it does not undergo cleavage. This is suggested by the fact that there is no production of 14CO2 after administration of HMM-ring-14C to either man or rats. The identification of the major urinary metabolites as methylmelamines and melamine also confirms the stability of the s-triazine ring in mammalian systems. The results of our experiments show that any metabolites formed from the opening of the s-triazine ring of HMM	REACH registration data	Reliability 2 Not according to any guideline, sufficiently good description of the method.

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
		in man or rats would be present in small quantities only.		
	Other	No data located		
Acute mammalian toxicity		**LOW:** Based on an oral LD50 > 2000 mg/kg bw for male and female rats.		
Acute lethality	Oral	LD50 > 2000 mg/kg bw for male and female rats Interpretation: practically nontoxic	REACH registration data	Reliability 1 GLP and guideline compliant study with well-characterized sample.
	Dermal	Data waiving	REACH registration data	
	Inhalation	LC50 > 5190 mg/m³ air (analytical), exposure duration 4 hours. No mortalities during exposure to the test item or during the observation period.	REACH registration data	Reliability 2 GLP and OECD testing guideline compliant study. It is acceptable to use the data of melamine for melamine phosphate because phosphate is not relevant for acute systemic toxicity.
Carcinogenicity		**MODERATE:** Based on read-across with melamine.		
	QSAR results from the literature (e.g. Danish QSAR database)	No data located		
	Carcinogenicity (Rat and Mouse)	Read-across with melamine (CAS No. 108-78-1). Carcinogenesis Bioassay of Melamine in F344/N Rats and B6C3F1 Mice (Feed Study). Duration of treatment 103 weeks, doses of: male rats 2250; 4500 ppm (ca. 150; 300 mg/kg bw/day), female rats: 4500; 9000 ppm (ca. 300; 600 mg/kg bw/day) Incidences of urinary bladder and kidney lesions, as well as tumour incidences were observed in the urinary bladder, pancreatic islets, thyroid and uterus.	REACH registration data	Reliability 2 Comparable to guideline study with acceptable restrictions (only two dose levels tested), study with melamine

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
		NOAEL carcinogenicity 2250 ppm for male rats NOAEL carcinogenicity 4500 ppm for female rats		
	Combined Chronic Toxicity/Carcinogenicity	No data located		
	Other	Melamine is not classifiable as to its carcinogenicity to humans (Group 3).	IARC Monograph	
		MODERATE hazard designation for carcinogenicity: Estimated based on the dissolution product melamine. There is experimental evidence that oral melamine exposure causes carcinogenicity in animals; however, no data were located to support its carcinogenicity in humans. Tumour formation in animals appeared to happen in a mechanical nature under conditions in which it produced bladder calculi.	US EPA, 2014	Report using the GreenScreen® methodology for an alternatives assessment for the flame retardant decabromodiphenyl ether (decaBDE).
Genotoxicity		**LOW:** Based on negative results in bacterial reverse mutation assays and micronucleus assays		
	Gene Mutation in vitro	Bacterial Reverse Mutation Assay, Negative, in *Salmonella typhimurium* strains TA-1535, TA-1537, TA-1538, TA-98, and TA-100, with and without metabolic activation. Bacterial Reverse Mutation Assay, Negative, in *E. coli WP2 uvr A*, with and without metabolic activation.	REACH registration data	Reliability 1 GLP and OECD guideline compliant study.
	Gene Mutation in vivo	No data located		
	Chromosomal Aberrations in vitro	No data located		
	Chromosomal Aberrations in vivo	Micronucleus assay on chromosome aberration in male mouse via intraperitoneal administration. Negative.	REACH registration data	Reliability 2 Comparable to guideline study with acceptable restrictions
	DNA Damage and Repair	No data located		

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Other			
Reproductive effects		**LOW:** Based on read-across with melamine.		
	Reproduc-tion/Developmental Toxici-ty Screen	No data located		
	Combined Repeated Dose with Reproduction/ Devel-opmental Toxicity Screen	No data located		
	Reproduction and Fertility Effects	Read across with melamine: Study details not provided. There was no evidence of adverse effects on reproductive organs - mammary glands, ovaries, prostate, seminal vesi-cles, testes and uterus (macroscopic and microscopic exami-nation) - from 13-week or carcinogenicity studies with rats and mice.	REACH registra-tion data for mel-amine	Reliability 2 NTP studies are of known high reliability.
	Other	Data for the melamine component support a low hazard designation.	US EPA, 2014	Report using the GreenScreen® methodology for an alternatives assessment for the flame retardant decabromodiphenyl ether (decaBDE).
Developmental effects		**LOW:** Based on read-across with melamine.		
	Reproduction/ Develop-mental Toxicity Screen	No data located		
	Combined Repeated Dose with Reproduction/ Devel-opmental Toxicity Screen	No data located		
	Prenatal Development	Read across with melamine: Wistar rats were exposed continuously to ca. 136; 400; 1060 mg/kg bw/day during post coitum days 6 - 16 (= 11 days) NOAEL maternal toxicity ca. 400 mg/kg bw/day	REACH registra-tion data	Reliability 2 Guideline Study (according to the former OECD 414 - exposure time from gd6-20) performed with melamine

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
		NOAEL teratogenicity >= 1060 mg/kg bw/day		
	Postnatal Development	No data located		
	Prenatal and Postnatal Development	No data located		
	Developmental Neurotoxicity	No data located		
	Other	For melamine, no adverse effects on gestational parameters, no signs of developmental toxicity have been reported.	US EPA, 2014	Report using the GreenScreen® methodology for an alternatives assessment for the flame retardant decabromodiphenyl ether (decaBDE).
Neurotoxicity		**No data located**		
	Neurotoxicity Screening Battery (Adult)	No data located		
	Other	No data located		
Repeated Dose Effects		**MODERATE:** Based on read-across with melamine, oral LOAEL for urinary bladder stones in male rats of 72 mg/kg bw/day.		
	Oral	Subchronic study with male and female Fischer 344 rats exposed for 13 weeks to: First study males 0, 560, 850, 1100, 100, 1700 mg/kg/day; females 0, 560, 880, 1200, 1400, 1600 mg/kg/day. Second study males 0, 72, 150, 300, 590, 1300 mg/kg/day; females 0, 84, 150, 300, 600, 1300 mg/kg/day NOAEL formation of urinary bladder stones and reduced body weights in female rats: 1400 mg/kg bw/day, LOAEL urinary bladder stones in male rats: 72 mg/kg bw/day	REACH registration data	Reliability 2 Read-across from supporting substance. Meets generally accepted scientific standards, well documented and acceptable for assessment, performed with melamine

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Oral	Male rats were exposed for 28 days at doses of 0; 2000; 4000; 7000; 10000; 13000; 16000; 19000 ppm (equivalent to ca. 200 - 1900 mg/kg bw/day). NOAEL urinary tract calculi 240 mg/kg bw/day	REACH registration data	Reliability 2 Read-across from supporting substance. Well-reported non-standard study, performed with melamine
	Oral	Subchronic study with male and female Fischer 344 rats exposed for 13 weeks to 0, 10000, 18000 ppm (plus 1% ammonium chloride in drinking water). LOAEL male/female (effect not specified) 1600 mg/kg bw/day	REACH registration data	Reliability 2 Read-across from supporting substance. Meets generally accepted scientific standards, well documented and acceptable for assessment, performed with melamine
Skin Sensitization		**LOW:** Based on negative results in Guinea pig maximisation test with melamine.		
	Skin Sensitization	Guinea pig maximisation test, intradermal and epicutaneous induction exposure with readings after 24 and 48 hours. No positive skin reaction in any animal at any reading time. Interpretation of results: not sensitising	REACH registration data	Reliability 2 GLP and OECD guideline compliant study with melamine.
Respiratory Sensitization		NO DATA LOCATED		
	Respiratory Sensitization	No data located		
Eye Irritation		NO DATA LOCATED		
	Eye Irritation	No data located		
Dermal Irritation		**LOW**: Based on negative results in an Acute Dermal Irritation / Corrosion study with melamine in rabbits.		
	Dermal Irritation	A skin irritation study with rabbits according to EU-, OECD- and EPA-methods was performed. Exposure to melamine resulted in no skin irritation in the treated skin-areas of the 6 rabbits. No signs of systemic intoxication were observed during the study period. Dermal application of melamine resulted in a primary irritation	REACH registration data for melamine	Reliability 1 Guideline study with GLP.

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
		index of 0 (non-irritating), when applied to the intact rabbit skin.		
Endocrine Activity		No data located		
		No data located		
Immunotoxicity		NO DATA LOCATED		
	Immune System Effects	No data located		

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7			
Property/Endpoint	**Data**	**Reference**	**Comments**
Ecotoxicity			
ECOSAR Class	Anilines (amino-meta), Melamines		
Aquatic Acute Toxicity	**LOW:** Two fish studies, including 5 species, with melamine are available, but no mortality occurred (mortality was not the primary effect tested) and LC50 values have therefore not been determined. Experimental data on algae exposed to melamine yield an EC50 > 325 mg/L. QSAR estimates on alga toxicity yield EC50 > 100 mg/L for the structural similar compound class of anilines. Based on the experimental data, a low hazard score is applied.		
Fish LC_{50}	96 h, LC50 3.3 * 10^5 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	ECOSAR version 1.11	
	96 h, LC50 15254 mg/L (Estimated) ECOSAR: Melamines	ECOSAR version 1.11	
	Fish (and pig and cat) were fed melamine and/or cyanuric acid for 3 days, to investigate induced renal crystals. Test organisms: 75 fish (21 tilapia, 24 rainbow trout, 15 channel catfish, and 15 Atlantic salmon) were used. None of the control fish or fish to which only melamine was administered had any clinical signs of distress, nor were any gross lesions detected during necropsies. No crystals were detected in any fish kidneys from control fish or fish to which only melamine was administered.	REACH registration data for melamine	Reliability 2 Acceptable publication without GLP.
	The aim of the study was to examine the pathological effects of feeding melamine (or cyanuric acid, separately or in combination) to walking catfish (140 fish). Exposure: 2 weeks, nominal concentrations concerning melamine alone: 0 (group 1) - 0.5 (group 2) - 2 % (group 4) melamine in the feed. The catfish developed darkening of the skin as early as 3	REACH registration data for melamine	Reliability 2 Acceptable, not well-documented publication without GLP.

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7			
Property/Endpoint	**Data**	**Reference**	**Comments**
	days post feeding. None of the catfish died during the 2-week experiment. Melamine-related crystals were not detected in fish, fed melamine alone.		
Daphnid LC_{50}	Static freshwater test with melamine in *Daphnia magna* exposed to nominal concentrations of 0 mg/L, 56 mg/L, 100mg/L, 180 mg/L, 320 mg/L, 560 mg/L, and 1000 mg/L 48 h, LC50 > 1000 mg/L (nominal) 24 h, LC50 > 1000 mg/L (nominal) 48 h, EC50 (mobility and behaviour) 200 mg/L (nominal) 24 h, EC50 (mobility and behaviour) 400 mg/L (nominal) 48 h, NOEC (mobility and behaviour) < 56 mg/L (nominal)	REACH registration data	Reliability 1 Guideline study with GLP on melamine
Green Algae LC_{50}	96 h, EC50 21.8 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	ECOSAR version 1.11	
	96 h, EC50 15969 mg/L (Estimated) ECOSAR: Melamines	ECOSAR version 1.11	
	Static freshwater test with melamine in *Pseudokirchnerella subcapitata* Nominal Concentrations: Control, 1000 ppm, 320 ppm, 100 ppm, 32 ppm and 10 ppm. 96 h, EC50 (area under the growth curve) > 325 mg/L (nominal)	REACH registration data for melamine	Reliability 2 A old study with GLP, but with poor description of the methods. No analytical determination of the concentrations used.
Aquatic Chronic Toxicity	**LOW:** Based on the lowest available NOEC for melamine, which is a NOEC in *Daphnia magna* of 18 mg/L.		
Fish NOEC	A semi-static test of the subacute effects of melamine to	REACH registra-	Reliability 2

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7			
Property/Endpoint	**Data**	**Reference**	**Comments**
	juvenile fish of Rainbow trout (*Oncorhynchus mykiss*) was conducted over a 28 day period at concentrations of 0, 750, 1500, and 3000 ppm. NOEC weight 1500 mg/L, nominal concentration NOEC mortality 1500 mg/L, nominal concentration LC50 mortality >3000 mg/L, nominal concentration	tion data	Well-documented study report, conducted with a method similar to present guidelines.
	260 mg/L, Fish ChV	PBTprofiler.net	QSAR estimation
Daphnid NOEC	Chronic toxicity and reproduction semi-static test to *Daphnia magna* exposed to melamine for 7 - 21 d at concentrations of 100, 180, 320, 560, 1000 and 1800 mg/L (first test), 10, 18, 32, 56 and 100 mg/L (second test), and 5.6, 10, 18, 32 and 56 mg/L (third test). 7 d, LC50 > 32 < 56 mg/L, nominal 21 d, LC50 > 32 < 56 mg/L, nominal 21 d, NOEC reproduction 18 mg/L, nominal 21 d, NOEC mortality 18 mg/L, nominal	REACH registration data	Reliability 2 Old study (1978) and short description in the report. Method similar to OECD guideline. No analytical determination of the test media concentrations.
Green Algae NOEC	Algal growth inhibition test with *Pseudokirchneriella subcapitata* exposed to 1000ppm, 320ppm, 100ppm, 32ppm and 10 ppm 96 h, EC50 area under the growth curve 325 mg/L nominal 96 h, NOEC (effect not specified) 98 mg/L nominal. Conclusion: The toxicity of melamine to algae, as measured by growth inhibition, is low.	REACH registration data	Reliability 2 A old study (1988) with GLP, but with poor description of the methods. No analytical determination of the concentrations used.
Transport	Results of Level III fugacity modelling indicate that at equilibrium the substance will be found exclusively in water (25%) and soil (75%). The expected mobility in soil is high, based on an estimated log Koc of 1.31 – 1.51. The Henry's Law Constant indicates that the substance will not		

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
		volatilise from the water surface.		
	Henry's Law Constant (atm m^3/mol)	0 (QSAR)	REACH registration data	Reliability 2 QSAR-method used by US EPA on melamine.
	Sediment/Soil Adsorption/Desorption – K_d/K_{oc}	$logK_{oc}$ = 1.13 (1) $logK_{oc}$ = 1.51 (2)	REACH registration data	Reliability 2 Two QSAR estimations are performed on melamine. One is described in the EU Technical Guidance Document (1), the other is used by the UDS EPA (2).
	Level III Fugacity Model	Water 25% Soil 75% Sediment 0% Air 0%	PBTprofiler.net	QSAR estimation
Persistence		**VH:** Experimental data show that melamine is not readily biodegradable in neither water nor soil. QSAR-estimates support the experimental data. The estimated half-life of 340 days in sediment leads to the very high hazard designation.		
Water	Aerobic Biodegradation	Ready Biodegradability test on melamine. 0 % Degradation after 2 weeks (activated sludge). Melamine is not readily biodegradable.	REACH registration data	Reliability 2 Database source, only few details are provided, but database is created and used by the Japanese authorities, and is therefore considered to be sufficiently reliable.
	Volatilization Half-life for Model River	No data located		
	Volatilization Half-life for Model Lake	No data located		
	Half-Life Water	38 days	PBTprofiler.net	QSAR estimation
Soil	Aerobic Biodegradation	Degradation of melamine was measured in a silty clay loam (soil 1, pH 8.2, initial concentration 2000 and 230 mg/kg soil) for 28 weeks and in a sandy loam (soil 2, pH 5.2, initial concentration 230 mg/kg soil) for 24 weeks. Soil 1:	REACH registration data	Reliability 2 Publication, which meets basic scientific principles, but which is rather old (1964) and not well described.

<table>
<tr><th colspan="5">1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7</th></tr>
<tr><th colspan="2">Property/Endpoint</th><th>Data</th><th>Reference</th><th>Comments</th></tr>
<tr><td colspan="2"></td><td>
<table>
<tr><th>Weeks</th><th>% Degr.</th><th>Parameter</th></tr>
<tr><td>6</td><td>6.4</td><td>nitrification; solution</td></tr>
<tr><td>6</td><td>7.7</td><td>nitrification; powder</td></tr>
<tr><td>10</td><td>0.7</td><td>nitrification; % of organic N, found as NO3- N; granules.</td></tr>
<tr><td>12</td><td>9.1</td><td>nitrification; solution</td></tr>
<tr><td>12</td><td>9.1</td><td>nitrification; powder</td></tr>
<tr><td>18</td><td>10.5</td><td>nitrification; solution</td></tr>
<tr><td>18</td><td>15.4</td><td>nitrification; powder</td></tr>
<tr><td>24</td><td>13.7</td><td>nitrification; solution</td></tr>
<tr><td>24</td><td>17.9</td><td>nitrification; powder</td></tr>
<tr><td>28</td><td>0</td><td>nitrification; granules</td></tr>
</table>
Soil 2:
<table>
<tr><th>Weeks</th><th>% Degr.</th><th>Parameter</th></tr>
<tr><td>6</td><td>0</td><td>nitrification; powder</td></tr>
<tr><td>12</td><td>0</td><td>nitrification; powder</td></tr>
<tr><td>18</td><td>3.9</td><td>nitrification; powder</td></tr>
<tr><td>24</td><td>8.9</td><td>nitrification; powder</td></tr>
</table>
</td><td></td><td></td></tr>
<tr><td colspan="2">Anaerobic Biodegradation</td><td>No data located</td><td></td><td></td></tr>
<tr><td colspan="2">Soil Biodegradation with Product Identification</td><td>No data located</td><td></td><td></td></tr>
<tr><td colspan="2">Sediment/Water Biodegra-dation</td><td>No data located</td><td></td><td></td></tr>
<tr><td colspan="2">Half-life soil</td><td>75 days</td><td>PBTprofiler.net</td><td>QSAR estimation</td></tr>
<tr><td colspan="2">Half-life sediment</td><td>340 days</td><td>PBTprofiler.net</td><td>QSAR estimation</td></tr>
<tr><td>Air</td><td>Atmospheric Half-life</td><td>24 days</td><td>PBTprofiler.net</td><td>QSAR estimation</td></tr>
</table>

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
Reactivity	Photolysis	No data located		
	Hydrolysis	No data located		

1,3,5-triazine-2,4,6-triamine phosphate/ CAS No. 41583-09-9/ EC no. 255-449-7				
Property/Endpoint		**Data**	**Reference**	**Comments**
Environmental Half-life		No data located		
Bioaccumulation		**VL:** Based on measured BCF values for melamine < 100.		
	Fish BCF	Flow-through test with melamine on *Cyprinus carpio*, 6 week exposure at 2 mg/L and 0.2 mg/L. BCF at 2 ppm < 0.38 BCF at 0.2 ppm < 3.8	REACH registration data	Reliability 2 Database source, only few details are provided, but database is created and used by the Japanese authorities, and is therefore considered to be sufficiently reliable.
	Fish BCF	Static test with melamine on *Pimephales promelas*, 96 and 72 h exposure. BCF at 0.082 mg/L < 0.48 (96 h, basis viscera) BCF at 0.082 mg/L < 0.26 (96 h, basis carcass)	REACH registration data	Reliability 2 Old (1984) but reasonably well described study. Similar to present guidelines.
	Fish BCF	Determination of BCF after static exposure of *Oncorhynchus mykiss* to melamine for 72 h. BCF at 0.089 mg/L < 0.11 (72 h, basis viscera) BCF at 0.089 mg/L < 0.26 (72 h, basis muscle) BCF at 0.091 mg/L < 0.11 (64 h, basis viscera) BCF at 0.091 mg/L < 0.03 (64 h, basis muscle)	REACH registration data	Reliability 2 Old (1984) but reasonably well described study. Similar to present guidelines.
	Other BCF	3.2	PBTprofiler.net	QSAR estimation
	BAF	No data located		
	Metabolism in Fish	No data located		
Environmental biomonitoring				
Ecological Biomonitoring		No data located		
Human Biomonitoring		Recoveries of melamine ranged between 90.3 +/- 7.8 and 102.1 +/- 5.6% at levels of 0.6 to 2.4 ppm in 4 kinds of beverages. The quantitation limit was 2.5 micrograms melamine in 50 mL beverage.	REACH registration data	Reliability 2 Documented analytical method. No GLP.

BASF, 2010: Technical data sheet for Melapur® MP.

ECOSAR/EPI (EPIWIN/EPISUITE) Estimations Programs Interface for Windows, Version 1.11. U.S. Environmental Protection Agency: Washington D.C. http://www2.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model

IARC Monograph: Melamine. Available at: monographs.iarc.fr/ENG/Monographs/vol73/mono73-17.pdf

Metadynea, 2014: Technical data sheet MPT11, 1,3,5-Triazine-2,4,6-triaminephosphate.

PBTprofiler.net: US EPA PBT Profiler, Model tool available at http://www.pbtprofiler.net/, search termes CAS No.: 41583-09-9, Name: 1,3,5-triazine-2,4,6-triamine phosphate, SMILES: n1c(N)nc(N)nc1N P(=O)(O)(O)O

REACH registration data: http://echa.europa.eu/da/information-on-chemicals/registered-substances using CAS No. 41583-09-9 as search term.

US EPA (2014). An alternatives assessment for the flame retardant decabromodiphenyl ether (decaBDE). US Environmental Protection Agency.

Appendix 8 Ethylenediamine phosphate, CAS No. 14852-17-6

Ethylenediamine phosphate consists of a mixture of ethylenediamine and phosphoric acid. Ethylenediamine (CAS No. 107-15-3) is therefore used as chemical surrogate in case of lack of data for ethylenediamine phosphate.
Ethylenediamine has a harmonised classification comprising the following health hazards: Acute Tox. 4 * (H302), Acute Tox. 4 * (H312), Skin Corr. 1B (H314), Skin Sens. 1 (H317), Resp. Sens. 1 (H334). Phosphoric acid (CAS No. 7664-38-2) also has a harmonised classification: Skin Corr. 1B (H314).

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9			
Property/Endpoint	**Data**	**Reference**	**Comments**
Physical/chemical properties			
Melting Point (°C)	325 °C There was no decomposition & sublimation observed of ethylenediamine, salt with phosphoric acid at the melting point.	REACH registration data	Reliability 1
	Decomposition starts at (°C) 230	Metadynea, 2014	No study details provided
Boiling Point (°C)	340 °C No decomposition of ethylenediamine, salt with phosphoric acid was observed at the boiling point.	REACH registration data	Reliability 1
Vapour Pressure (Pa)	0.000000034 Pa at 25 °C	REACH registration data	Reliability 2 estimated by calculation
Water Solubility (mg/L)	3000 mg/L	REACH registration data	Reliability 1
	50 g/L (for commercial product)	Metadynea, 2014	No study details provided
Log Kow	-2.522 at 28 °C and pH of 6.69	REACH registration data	Reliability 1
pKa	0.2760×10^{-12}	REACH registration data	

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
Human health effects				
Toxicokinetics		Based on the available studies, the substance appears to have low bioaccumulation potential. Ethylenediamine (EDA) is readily absorbed after oral and respiratory administration in animal models. Absorption was rapid as the EDA concentration in plasma reached a maximum at about 1 hour after dosing in mice. EDA is distributed throughout the body, with the liver and kidney attaining the highest concentration among the major organs. Urine is the major route of excretion (ca. 45 – 55 %), smaller fractions (ca. 4 – 16% and 6 – 8%, respectively) are excreted via faeces and respiration, and excretion was quite rapid. The principle metabolite in the urine was N-acetylethylenediamine.		
Dermal absorption *in vitro*		No data located.		
Absorption, Distribution, Metabolism & Excretion	Oral, dermal or inhaled	Read- across with ethylenediammonium dichloride (CAS No. 333-18-6): Metabolism and pharmacokinetics of ethylenediamine in the rat following oral, endotracheal or intravenous administration. Doses: 5, 50 and 500 mg/kg bodyweight, 24 or 48 hours study of distribution following single dose. Results: Rapid absorption from gastrointestinal as well as from respiration tract. Distributed in body, but liver, kidneys, thyroid and bone marrow contained highest concentrations. Excretion via urine: 45-55%, faeces: 4-16%, CO2: 6-8%. Interpretation of the results: low bioaccumulation potential based on study results	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 No data on GLP, study from 1982.
		Read- across with ethylenediammonium dichloride (CAS No. 333-18-6): Oral gavage, endotracheal or intracardial administration of EDA*2HCl in male mice. Doses: 5, 50 and 500 mg/kg bodyweight, 48 hours study of distribution following single dose. Results:	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 No data on GLP, study from 1982.

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		Readily absorbed from the gut, bioavailability, 87% measured at 50 mg/kg. Rapid absorption, EDA concentration in plasma reached a maximum 1 h after dosing. Distributed throughout the body, with the liver and kidney attaining the highest concentration among the major organs. Excretion via urine was the major route of excretion >50 %. Faecal: 4-13 %, respiratory: 8%. Excretion was rapid > 70% eliminated within 24 h. Clearance and terminal half-life varies only slightly depending on route of administration. Interpretation of the results: low bioaccumulation potential based on study results		
	Other	Absorption through inhalation is not considered a relevant exposure pathway due to the low vapour pressure of the substance. Based upon the physico-chemical properties and BCF of ethylenediamine, salt with phosphoric acid, it has been deduced that the chemical has potentially low bio-accumulative property and hence shall be eliminated from the body system through urine or faeces.	REACH registration data	Reliability 2 Based on the weight of evidence of various physical- chemical and bioaccumulative parameters in the dossier
Acute mammalian toxicity		**LOW:** Based on the oral and dermal LD50 > 2000 mg/kg bw for female rats.		
Acute lethality	Oral	Oral exposure study with Wistar rats according to OECD Guideline 423. LD50 > 2000 mg/kg bw for female rats	REACH registration data	Reliability 1 according to OECD Guideline 423
	Dermal	Dermal exposure study with Wistar rats according to OECD Guideline 402 (Acute Dermal Toxicity). The test compound CAS No. 14852-17-6 when applied dermally at the dose level of 2000 mg/kg b.wt. on Wistar albino rats	REACH registration data	Reliability 1 according to OECD Guideline 402

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		did not produce any mortality during the observation period of 14 days. LD50 > 2000 mg/kg bw for male/female rats		
	Inhalation	Data waiving due to exposure considerations	REACH registration data	
Carcinogenicity		**LOW:** Based on a carcinogenicity study with a chemical surrogate.		
	QSAR results from the literature (e.g. Danish QSAR database)	No data located.		
	Carcinogenicity (Rat and Mouse)	Read-across with ethylenediammonium dichloride (CAS No. 333-18-6). 2 Year oral exposure study with Fischer 344 rats, exposure every 2nd week in dose groups of 20, 100, and 350 mg/kg bw. 10 rats/sex/dose and control group were scheduled for sacrifice at 6 and 12 month, 20 rats/sex/dose and control group were scheduled for sacrifice at 18 month. NOAEL carcinogenicity 159 mg/kg bw/day (actual dose received) There was no evidence of carcinogenic effects.	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 No GLP data
	Combined Chronic Toxicity/Carcinogenicity	No data located.		
Genotoxicity		**LOW:** Based on negative results in the bacterial reverse mutation assay and QSAR estimations for ethylenediamine phosphate and the conclusion on genotoxicity for ethylenediamine.		
	Gene Mutation *in vitro*	Bacterial reverse mutation assay: The Salmonella Mutagenicity Test is negative with and without metabolic activation.	REACH registration data	Reliability 2 Authoritative data base
		QSAR Toolbox 2.3.0.1132 prediction for "Gene Mutation" read across evaluation for 14852-17-6	REACH registration data	Reliability 2 Prediction report

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		The prediction is done for ethylenediamine, salt with phosphoric acid for *S. typhimurium* TA 1535, TA 1537, TA 98 and TA 100 for genetic toxicity without metabolic activation. The substance is estimated to be negative.		
	Gene Mutation *in vivo*	No data located.		
	Chromosomal Aberrations *in vitro*	QSAR Toolbox 2.3.0.1132 prediction for "Chromosome Aberration" read across evaluation for 14852-17-6 The prediction is done for ethylenediamine, salt with phosphoric acid for Chinese Hamster Lungcell for genetic toxicity with metabolic activation is estimated to be negative.	REACH registration data	Reliability 2 Prediction report
	Chromosomal Aberrations *in vivo*	No data located.		
	DNA Damage and Repair	No data located.		
	Other	SIDS Initial Assessement Profile on ethylenediamine. Conclusion on review of eight genotoxicity studies: *The weight of evidence from both in vitro and in vivo tests indicates that ethylenediamine is unlikely to be genotoxic. It was also negative in chronic bioassays via two routes, oral and dermal.*	UNEP, 2001	
Reproductive effects		**LOW:** Based on read-across with ethylenediammonium dichloride, resulting in a NOAEL of 500 mg/kg/day (highest dose given) in rats.		
	Reproduction/Developmental Toxicity Screen	Read-across with ethylenediammonium dichloride (CAS No. 333-18-6): In a two-generation study, male and female Fischer 344 rats were fed diets containing 0, 50, 150 or 500 mg/kg/day. There was no indication of reproductive toxicity in Fischer 344 rats, following exposure to dietary EDA for two generations, leading to a NOAEL of 500 mg/kg/day (highest dose given) in rats.	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 pre-GLP (1984)

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Continuous breeding study	No data located.		
	Combined Repeated Dose with Reproduction/Developmental Toxicity Screen	QSAR Toolbox Two-generation study in which 25 male and female rats were studied at doses 5, 10 and 25 mg/kg/day. LOEL for the F2 Generation (male/female) 35.46 mg/kg bw/day (effect: Pituitary Pathology and Weight)	REACH registration data	Reliability 2 Prediction report
	Reproduction and Fertility Effects	No data located.		
	Other	No data located.		
Developmental effects		**Moderate:** Based on weight of evidence from available studies with ethylenediammonium and ethylenediammonium dichloride. A single study in rats noted reduction of body weight gain and diet consumption, decreased number of live foetuses/litter and increased number of resorptions/litter in dams receiving 1000 mg/kg/day, these effects are most likely due to maternal toxicity. None of the studies identified teratogenic effects. A NOAEL for maternal toxicity ≥ 80 mg/kg bw/day (highest dose tested) was identified in two rabbit studies. The score "moderate" is assigned based on a conservative approach due to maternal toxicity.		
	Reproduction/Developmental Toxicity Screen	QSAR Toolbox Developmental Study in which 25 female rats were studied at doses 5, 10 and 25 mg/kg/day LOEL fetotoxicity 106.44 mg/kg bw/day	REACH registration data	Reliability 2 Prediction Report
		Read-across with ethylenediammonium dichloride (CAS No. 333-18-6). In a gavage study ten Fischer 344 rats were fed ethylenediamine di-hydrochloride by gavage 1000 mg/kg/day on gestation day 6-15. The aim was to decide if this dose by gavage would reduce diet consumption, similar to results shown in a diet study. Reduction of body weight gain and diet consumption, decreased number of live foetuses/litter and increased number of resorptions/litter were noted.	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 pre-GLP (1987)
		Read-across with ethylenediammonium dichloride (CAS No. 333-18-6). Rats were administered a dietary dose of 1000 mg/kg/day on	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 pre-GLP (1984)

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		gestation day 6- 15. The results of these studies indicate that ethylenediamine dihydrochloride was not teratogenic in the Fischer 344 rat.		
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Oral exposure study with New Zealand White rabbits exposed to 0, 10, 40 or 80 mg/kg/day. The maternal and developmental NOAEL for EDA in the New Zealand White rabbit exposed during major organogenesis is greater than or equal to 80 mg/kg/day. Higher doses were not evaluated in this study due to the observation of greater than or equal to 20% maternal mortality at greater than or equal to 100 mg/kg/day in a preliminary investigation. There were no treatment-related maternal deaths in this study, and no characteristic clinical signs of toxicity in EDA-treated dose. Uterine examination on gd 30 revealed no adverse effects of EDA upon prenatal viability, litter size, fetal weight or fetal morphology. NOAEL maternal toxicity ≥ 80 mg/kg bw/day (highest dose tested)	REACH registration data	Reliability 2 Authoritative data base, NTP Study: TER92020, 2012, according to Guideline EPA OPPTS 870.3700
		Read-across with ethylenediammonium (EDA) dichloride (CAS No. 333-18-6). Rabbits were dosed during gestation days 6 - 19. On day 21 uterine contents are examined, and the foetuses are evaluated for externally visible anomalies and for soft tissue and skeletal changes. Maternal examinations were fetal growth, viability and morphological development. NOAEL maternal toxicity ≥ 80 mg/kg bw/day (highest dose tested) No characteristic clinical signs of toxicity were observed. No effect on maternal food intake, body weight or weight gain,	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 No guideline followed, no information on GLP.

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		liver or kidney weight. No adverse effects on prenatal viability, litter size, fetal weight or fetal morphology was observed		
	Prenatal Development	No data located.		
	Postnatal Development	No data located.		
	Prenatal and Postnatal Development	No data located.		
	Developmental Neurotoxicity	No data located.		
	Other	No data located.		
Neurotoxicity		**DG**		
	Acute and delayed neurotoxicity tests in hens	No data located.		
	Other	No data located.		
Repeated Dose Effects		**MODERATE:** Based on a NOAEL of 22 mg/kg/day EDA and a NOEL of 20 mg/kg/day EDA in a 13-week and 2-year rat study, respectively.		
	Sub-chronic oral repeated dose	QSAR Toolbox Chronic Study with rats exposed at doses of 0.00, 7500.00, 15000.00 (unit not specified) for 540 days. LOEL (male/female) 966.34 mg/kg bw/day (body weight decreased)	REACH registration data	Reliability 2 Prediction Report
		Read-across with ethylenediammonium dichloride (CAS No. 333-18-6). In a three month dietary study, male and female rats were fed targeted doses of 0, 50, 250 or 1000 mg/kg/day EDA-2HCl. There were no deaths and no abnormal clinical signs noted during the study. Body weight gains were significantly decreased in the high dose group, which affected a number of absolute and relative organ weights in both males and females. Water consumption was comparable to control values at all	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 The study was performed pre-GLP. No guideline was available.

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		dose levels in males but was decreased in a dose-response manner in female rats at all 3 dose levels. Slight reductions in serum glucose levels and an elevation of alkaline phosphatase, AST and ALT activities were observed in the high dose group. An elevation of ALT activity was also observed in the intermediate dose male rats. Urinary pH in the high dose group was decreased in both males and females. There were no dose-related gross lesions in any animal on the study. The most significant histopathologic lesion, hepatocellular pleomorphism, was observed primarily in the high dose female and, to a lesser extent, male rats. LOAEL 114 mg/kg/day EDA (250 mg/kg/day EDA-2HCl) NOAEL 22 mg/kg/day EDA (50 mg/kg/day EDA-2HCl)		
		Review of seven dietary/oral gavage studies: *Conclusions: In repeated dose studies, decreased body weight and water and feed consumption have been observed and are probably related to the irritating nature of EDA and it's high pH.* *Hepatocellular pleomorphism has been observed in several dietary studies of varying duration. The lowest LOAEL was 100 mg/kg/day with a NOEL of 20 mg/kg/day in the chronic dietary feeding study* (two-year bioassay) .	UNEP, 2001	
	Sub-chronic inhalation repeated dose	No data located.		
	Dermal repeated dose	No data located.		
Skin Sensitization		**HIGH:** Based on harmonised classification of ethylenediamine. Since sub-category (1A or 1B) is not specified, we precautiously assign the score "high" (corresponding to sub-category 1A).		
	Skin sensitization	QSAR predictions by Danish EPA model, Guinea pig maximisation test or human experience.	REACH registration data	Reliability 2 Prediction model

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		Skin sensitisation potential of ethylenediamine, salt with phosphoric acid is estimated to be positive.		
		QSAR Toolbox Version 2.3 prediction for "Skin Sensitisation" read across evaluation for 14852-17-6 Based on this prediction it can be concluded that ethylenediamine, salt with phosphoric acid is classified as skin sens.1 as per the criteria of CLP regulation.	REACH registration data	Reliability 2 Prediction model
		Notified classification and labelling according to CLP criteria (8 notifiers) Skin Sens. 1	ECHA C&L inventory	
		Advisory health classification: SkinSens1	Danish Environmental Protection Agency	
		Skin Sens. 1 (H317 - May cause an allergic skin reaction). Sub-category (1A or 1B) is not specified, possibly due to insufficient data.	ECHA C&L inventory for ethylenediamine (CAS No. 107-15-3)	Harmonised classification
	Skin sensitization in humans	No data located.		
Respiratory Sensitization		**HIGH:** Based on harmonised classification of ethylenediamine. Since sub-category (1A or 1B) is not specified, we precautiously assign the score “high” (corresponding to sub-category 1A).		
	Respiratory Sensitization	Resp. Sens. 1 (H334)	ECHA C&L inventory for ethylenediamine (CAS No. 107-15-3)	
Eye Irritation		**LOW:** Based on guideline study.		
	Eye Irritation	Study on New Zealand White rabbits The eyes were examined at 1, 24, 48 and 72 hours after test substance application. The grades of ocular reaction (conjunctiva, cornea and iris) were recorded at each observation. To	REACH registration data	Reliability 1 OECD Guideline 405

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		determine the reversibility of the effect the animal was observed normally for 21 days. Practically not irritating effects were fully reversible. Interpretation of results: not irritating		
Dermal Irritation		**VH:** Based on harmonised classification for ethylenediamine and phosphoric acid.		
	Dermal Irritation	Study on New Zealand White rabbits Skin reaction The test compound CAS No. – 14852-17-6 applied at the dose level of 0.5 gm on shaven back skin (approximately 6 cm^2) of rabbit did not produce any clinical signs of irritation to skin during period of observation. The duration of application of test compound was 24th hour and the observation period 14 days. Conclusion: not irritating	REACH registration data	Reliability 1 OECD Guideline 404
		Skin Corr. 1B (H314 - Causes severe skin burns and eye damage)	ECHA C&L inventory for ethylenediamine (CAS No. 107-15-3)	
		Skin Corr. 1B (H314 - Causes severe skin burns and eye damage)	ECHA C&L inventory for phosphoric acid (CAS No. 7664-38-2)	
Endocrine Activity		**DG**		
	Endocrine activity	No data located.		
Immunotoxicity		**DG**		
	Immune System Effects	No data located.		

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9			
Property/Endpoint	**Data**	**Reference**	**Comments**
Ecotoxicity			
ECOSAR Class	Aliphatic Amines		
Aquatic Acute Toxicity	**MODERATE:** Based on an EC50 of 16.7 mg/L for *Daphnia magna*.		
Fish LC_{50} (Freshwater)	Short term toxicity to fish by ECOSAR Version 1.10 96 h, LC50 24,0000 mg/L	REACH registration data	Reliability 2 Prediction model
	QSAR Toolbox 2.3.0.1132 prediction for LC50 read across evaluation on *Oncorhynchus mykiss* 96 h, LC50 203.3 mg/L	REACH registration data	Reliability 2 Prediction model
	Study on ethylenediammonium (EDA). Semi-static test with *Poecilia reticulata* exposed to 0, 180, 320, 560, 1000, and 1800 mg/l nominal concentrations. 96 h, LC50 640 mg/L	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Study performed under GLP and according to guidelines (EU Method C.1). No analytical monitoring was performed.
Fish LC_{50} (Marine)	No data located.		
Daphnid LC_{50} / EC_{50} (Freshwater)	Short term toxicity to aquatic invertebrates by ECOSAR Version 1.10 on *Daphnia magna* 48 h, LC50 6266.7 mg/L	REACH registration data	Reliability 2 Prediction model
	QSAR Toolbox 2.3.0.1132 prediction for EC50 read across evaluation on *Daphnia magna* 48 h, EC50 191 mg/L	REACH registration data	Reliability 2 Prediction model
	Study on ethylenediammonium (EDA). *Daphnia magna* exposed to 0, 5.6, 10, 32, 56, and 100 mg/l nominal concentrations.	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Study performed under GLP and according to guidelines (EU Method C.2). No

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9			
Property/Endpoint	**Data**	**Reference**	**Comments**
	48 h, EC50, 16.7 mg/L		analytical monitoring was performed.
Daphnid LC_{50} / EC_{50} (Marine)	No data located.		
Green Algae IC_{50} / EC_{50}	Short term toxicity to aquatic algae by ECOSAR Version 1.10 on green algae 96 h, EC50 321 mg/L (growth rate)	REACH registration data	Reliability 2 Prediction model
	QSAR predictions by Danish EPA, Multicase model is used to estimate EC50 (growth) of algae *Pseudokirchneriella subcapitata* No details on exposure duration, EC50 386 mg/L (growth rate)	REACH registration data	Reliability 2 Prediction model
	Study on ethylenediammonium (EDA). *Pseudokirchneriella subcapitata* exposed to 0, 3.2, 10.2, 32.8, 104.9, and 335.5 mg/l nominal concentrations. 72 h, EC50 (biomass) 71 mg/L 72 h, EC50 (growth rate) 645 mg/L	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Study performed under GLP and according to according to EU Method C.3 (Algal Inhibition test) including updates published 1988. No analytical monitoring was performed.
Aquatic Chronic Toxicity	**HIGH:** Based on a 21 d NOEC of 0.16 mg/L for *Daphnia magna*.		
Fish NOEC (Freshwater)	Data waiving, study scientifically unjustified	REACH registration data	
	Study on ethylenediammonium (EDA). Semi-static test with *Gasterosteus aculeatus* on early-life stage: reproduction, (sub)lethal effects. A preliminary test was performed with the following concentrations: 0, 1, 10, 50, 100, 300 mg/l . 10 eggs were used per concentration. On the basis of these results a limit test was performed at 10 mg/l, using 60 eggs.	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Study performed under GLP and according to OECD Guideline 210. No analytical monitoring was performed.

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		28 d, NOEC > 10 mg/L		
Daphnid NOEC (Freshwater)		Data waiving, study scientifically unjustified	REACH registration data	
		Study on ethylenediammonium (EDA). Semi-static test with *Daphnia magna* exposed to 0.08 -5 mg/L. 21 d, NOEC (reproduction rate) 0.16 mg/L	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Limited information on procedures, no GLP.
Green Algae NOEC		QSAR Toolbox 2.3.0.1132 prediction for NOEDC read across evaluation on *Pseudokirchneriella subcapitata* 72 h, NOEC 3.06 mg/L (growth)	REACH registration data	Reliability 2 Prediction model
		Study on ethylenediammonium (EDA). Static test with *Pseudokirchneriella subcapitata* exposed to 0, 3.2, 10.2, 32.8, 104.9, and 335.5 mg/l nominal concentrations. 72 h, NOEC 3.2 mg/L (growth rate)	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Study performed under GLP and according to according to EU Method C.3 (Algal Inhibition test) including updates published 1988. No analytical monitoring was performed.
Transport		The substance shows considerable water solubility. According to QSAR predictions, ethylenediamine-o-phosphate will be found primarily in the water compartment (78.1 %), with a smaller fraction in soil (21.8%) and very little in air (0.1%). In the atmosphere, the substance is expected to be present only associated with water aerosols and removal from air is therefore by wet deposition. Experimental data for EDA indicate relative immobility in soil (Koc = 4,786), and phosphates are known to sorb strongly to i.e. clay particles in soil.		
	Henry's Law Constant (atm-m^3/mole)	HENRYs LAW CONSTANT by EPI (Estimation Programs Interface) Suite 9.14 * 10^{-22} Pa m^3/mol	REACH registration data	Reliability 2 Prediction model
	Sediment/Soil Adsorption/Desorption – K_d/K_{oc}	Adsorption by EPI Suite Estimated via MCI method Koc=6.27; log koc=0.797	REACH registration data	Reliability 2 Prediction model
		Study on ethylenediammonium (EDA).	REACH registration data	Reliability 1

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
		Six different soils were used. Five were collected from the vadose zone: two sandy loams, a sandy clay loam, a silty loam, and a clay. The sixth soil was a sand collected from an aquifer. Conclusions: Batch equilibrium adsorption studies were conducted which showed a log Koc of 3.68 (Koc = 4,786), indicating relative immobility in soil.	for ethylenediamine (CAS No. 107-15-3)	equivalent or similar to OECD Guideline 106
	Level III Fugacity Model	Model for EDA: Using the default emissions of equal amount to soil, air and water (1000 kg/hour for each compartment), the percentage of ethylenediamine in bulk water, air and soil predicted by the Level III model are 78.1, 0.1 and 21.8% respectively. Regardless of the media to which EDA is released, most of the EDA at steady state is in the water phase. These results are consistent with the physical properties of EDA, namely the high water solubility and low air-water and octanol-water partition coefficients.	UNEP, 2001	
Persistence		**VERY LOW:** Based on biodegradation test with EDA (95 % degradation in 28 d) and QSAR estimations resulting in a half-life in water of 15 days and of 3.01 h due to biodegradation and hydrolysis, respectively.		
Water	Aerobic Biodegradation	Bio-degradation in water by Environmental Science Center's PBT profiler, ready biodegradability Half-life 15 days (readily biodegradable)	REACH registration data	Reliability 2 Prediction model
		Biodegradation in water by EPI (Estimation Programs Interface) Suite Half-life 15 days (readily biodegradable)	REACH registration data	Reliability 2 Prediction model
		Activated sludge, from an activated sludge plant, was used as inoculum. Ethylenediamine is degraded 95% in 28 days in the Closed Bottle Test and can be considered readily biodegradable.	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 1 according to EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test)

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Volatilization Half-life for Model River	No data located.		
	Volatilization Half-life for Model Lake	No data located.		
Soil	Aerobic Biodegradation	Bio-degradation in soil by Environmental Science Center's PBT profiler, ready biodegradability Half-life 30 days (readily biodegradable)	REACH registration data	Reliability 2 Prediction model
	Anaerobic Biodegradation	No data located.		
	Soil Biodegradation with Product Identification	No data located.		
	Sediment/Water Biodegradation	No data located.		
Other	Biotic degradation.	No data located.		
Air	Atmospheric Half-life	No data located.		
Reactivity	Photolysis	Phototransformation in air by Environmental Science Center's PBT profiler 50 % Degr. in air: 0.38 days	REACH registration data	Reliability 2 Prediction model
		Phototransformation by EPI (Estimation Programs Interface) Suite Half-life 6.08 h	REACH registration data for ethylenediamine (CAS No. 107-15-3)	Reliability 2 Prediction model
	Hydrolysis	Hydrolysis by EPI (Estimation Programs Interface) Suite Half-life 3.01 h	REACH registration data	Reliability 2 Prediction model

Ethylenediamine-o-phosphate /CAS No. 14852-17-6 /EC No. 238-914-9				
Property/Endpoint		**Data**	**Reference**	**Comments**
Environmental Half-life		No data located.		
Bioaccumulation		**VERY LOW:** Based on QSAR estimates resulting in BCFs << 100 and a measured log Kow << 3.		
	Fish BCF	Bioaccumulation by Environmental Science Center's PBT profiler, fish BCF 3.2 (non bioaccumulative)	REACH registration data	Reliability 2 Prediction model
		Bioaccumulation by EPI (Estimation Programs Interface) Suite, whole body, test organism not specified BCF 3.16 (non bioaccumulative)	REACH registration data	Reliability 2 Prediction model
	Other BCF	No data located.		
	BAF	No data located.		
	Metabolism in Fish	No data located.		
Environmental biomonitoring				
Ecological Biomonitoring		No data located.		
Human Biomonitoring		No data located.		

Danish Environmental Protection Agency, Database with QSAR predictions for classification: http://mst.dk/virksomhed-myndighed/kemikalier/stoflister-og-databaser/vejledende-liste-til-selvklassificering-af-farlige-stoffer/clp/ using CAS No. 14852-17-6 as search term.

ECHA C&L inventory: http://echa.europa.eu/information-on-chemicals/cl-inventory-database using CAS No. 14852-17-6 as search term.

Metadynea, 2014: EP11, Technical Data Sheet. November 2014.

REACH registration data: http://echa.europa.eu/da/information-on-chemicals/registered-substances using CAS No. 14852-17-6 as search term unless specified otherwise.

Appendix 9 6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide, CAS No. 848820-98-4

A notified classification is available for 6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide: Skin Irrit. 2 (H315; 29 notifiers), Aquatic Chronic 3 (H412; 28 notifiers), Acute Tox. 4 (H302, 1 notifier). The latter hazard statement is erroneous (there is no Category 4 for Acute Aquatic toxicity and H302 is a health hazard code) and is therefore disregarded.
Data for this substance were basically only available from the REACH registration data. QSAR estimates (from ECOSAR and PBT profiler) are therefore used to support available data and fill some of the data gaps.

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5			
Property/Endpoint	**Data**	**Reference**	**Comments**
Physical/chemical properties			
Boiling Point (°C)	Two experiments were conducted with the Siwoloboff method. No boiling point could be determined because of starting decomposition of the test item taking place at approx. 362 °C (635 K). Decomposition was indicated by a change of the colour of the test item, which became darker and finally red / brown during the tests.	REACH registration data	Reliability 1 OECD Guideline 103
	Decomposition starts at 250 °C	Metadynea, 2014	No further details
Vapour Pressure (Pa)	at 20 °C: $9.48 \cdot 10^{-8}$ Pa at 25 °C: $1.97 \cdot 10^{-7}$ Pa	REACH registration data	Reliability 1 OECD Guideline 104
Water Solubility (mg/L)	Mean water solubility at the plateau is 176.1 ± 5.9 mg/L.	REACH registration data	Reliability 1 OECD Guideline 105
Log Kow	3.32	REACH registration data	Reliability 1 OECD Guideline 117
	EPISuite WSKowwin v1.43 Estimate 3.390	ECOSAR v1.11	QSAR estimate
pKa	No data located.		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
Human health effects				
Toxicokinetics				
Dermal absorption *in vitro*		No data located.		
Absorption, Distribution, Metabolism & Excretion	Oral, dermal or inhaled	No data located.		
	Other	No data located.		
Acute mammalian toxicity		**LOW:** Based on a single oral dose of 2000 mg/kg, yielding no lethality, clinical symptoms, or changes in general state and behaviour.		
Acute lethality	Oral	No lethality was noted at single oral dose of 2000 mg/kg bw. No clinical symptoms were observed on the day of the treatment and during the 14-day observation period, the general state and behaviour of experimental animals were normal. The body weight development was undisturbed in all animals.	REACH registration data	Reliability 1 OECD Guideline 423
	Dermal	No data located.		
	Inhalation	No data located.		
Carcinogenicity		**DG**		
	QSAR results from the literature (e.g. Danish QSAR database)	No data located.		
	Carcinogenicity (Rat and Mouse)	No data located.		
	Combined Chronic Toxicity/Carcinogenicity	No data located.		
	Other	No data located.		
Genotoxicity		**DG**		
	Gene Mutation *in vitro*	Test results:	REACH registration data	Reliability 1

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
		Species/strain *Salmonella typhimurium* (TA 97a, TA 98, TA 100, TA 102 and TA 1535), with and without metabolic activation, Genotoxicity: negative Mutagenicity: No significant increase of the number of revertant colonies in the treatments with and without metabolic activation was observed. No concentration-related increase over the tested range was found. Therefore the test item is stated as not mutagenic under the test conditions.		OECD Guideline 471
	Gene Mutation *in vivo*	No data located.		
	Chromosomal Aberrations *in vitro*	No data located.		
	Chromosomal Aberrations *in vivo*	No data located.		
	DNA Damage and Repair	No data located.		
	Other	No data located.		
Reproductive effects		**DG**		
	Reproduction/Developmental Toxicity Screen	No data located.		
	Continuous breeding study	No data located.		
	Combined Repeated Dose with Reproduction/Developmental Toxicity Screen	No data located.		
	Reproduction and Fertility Effects	No data located.		
	Other	No data located.		
Developmental effects		**DG**		
	Reproduction/Developmental Toxicity Screen	No data located.		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	No data located.		
	Prenatal Development	No data located.		
	Postnatal Development	No data located.		
	Prenatal and Postnatal Development	No data located.		
	Developmental Neurotoxicity	No data located.		
	Other	No data located.		
Neurotoxicity		**DG**		
	Acute and delayed neurotoxicity tests in hens	No data located.		
	Other	No data located.		
Repeated Dose Effects		**DG**		
	Sub-chronic oral repeated dose	No data located.		
	Sub-chronic inhalation repeated dose	No data located.		
	Dermal repeated dose	No data located.		
Skin Sensitization		**LOW:** Based on results of a guideline study.		
	Skin sensitization	Mouse local lymphnode assay (LLNA): The test item KCCS DOB11 was not a skin sensitiser under the test conditions of this study.	REACH registration data	Reliability 1 OECD Guideline 429
	Skin sensitization in humans	No data located.		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
Respiratory Sensitization		**DG**		
	Respiratory Sensitization	No data located.		
Eye Irritation		**DG**		
	Eye Irritation	KCCS DOB11 induces effects on the cornea with an in vitro irritation score (IVIS) >3 and ≤ 55 . Therefore it cannot be classified in a UN GHS Category for eye damage. Because of the negative test result, a sequential testing strategy is necessary.	REACH registration data	Reliability 1 OECD Guideline 437
		No data located.		
Dermal Irritation		**HIGH:** Based on notified classification as Skin Irrit. 2 (H315) an irritation study with the human skin model EpiDermTM.		
	Dermal Irritation	Two tissues of the human skin model EpiDermTM were treated with KCCS DOB11 for three minutes and one hour, respectively. KCCS DOB11 is considered as not corrosive in the Human Skin Model Test.	REACH registration data	Reliability 1 OECD Guideline 431
		Three tissues of the human skin model EpiDermTM were treated with KCCS DOB11 for 60 minutes. KCCS DOB11 is considered as “irritant in the Human Skin Model Test”. In the UN GHS System for skin irritating substances, KCCS DOB11 should be classified in UN GHS category 2. KCCS DOB11 is considered as “irritant in the Human Skin Model Test”.	REACH registration data	Reliability 1 OECD Guideline 439
		Skin Irrit. 2 (H315: Causes skin irritation)	C&L inventory	Notified classification
Endocrine Activity		**DG**		
	Endocrine activity	No data located.		
Immunotoxicity		**DG**		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
	Immune System Effects	No data located.		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5			
Property/Endpoint	**Data**	**Reference**	**Comments**
Ecotoxicity			
ECOSAR Class	Esters (Phosphinates)		
Aquatic Acute Toxicity	**MODERATE:** A comparison of QSAR estimates for fish and crustaceans indicates that fish, for which experimental data are lacking, are less susceptible than crustaceans. At the same time, experimental data on daphnids and algae indicate that daphnids are less susceptible than algae. Furthermore, there is a large difference between the experimental and the estimated endpoint values for daphnids, the experimental study resulting in a much higher EC50 than the QSAR estimate. The acute aquatic toxicity score is therefore based on experimental data for algae with an EC50 (growth rate) of 13 mg/L.		
Fish LC_{50} (Freshwater)	Estimate for the ECOSAR class: Esters (Phosphinates) 96 h, LC50 1.96 mg/L	ECOSAR v1.11	QSAR estimate
Fish LC_{50} (Marine)	Estimate for the ECOSAR class: Esters (Phosphinates) 96 h, LC50 2.24 mg/L	ECOSAR v1.11	QSAR estimate
Daphnid LC_{50} / EC_{50} (Freshwater)	Semi-static test with *Daphnia magna* 24 h, EC50 (mobility) > 69 mg/L (nominal concentration) 48 h, EC50 (mobility) > 66 mg/L (nominal concentration)	REACH registration data	Reliability 1 OECD Guideline 202
	Estimate for the ECOSAR class: Esters (Phosphinates) 48 h, LC50 1.32 mg/L	ECOSAR v1.11	QSAR estimate
Mysid LC_{50} / EC_{50} (Marine)	Estimate for the ECOSAR class: Esters (Phosphinates) 96 h, LC50 0.255 mg/L	ECOSAR v1.11	QSAR estimate
Green Algae IC_{50} / EC_{50}	Test with *Desmodesmus subspicatus* 72 h, EC50 (growth rate) 13 mg/L (nominal concentration)	REACH registration data	Reliability 1 OECD Guideline 201
Aquatic Chronic Toxicity	**MODERATE**: Based on experimental data for algae with an EC10 (growth rate) of 4.2 mg/L considering that, based on the available information, algae appear to be more susceptible than fish and crusteans.		
Fish NOEC (Freshwater)	No data located.		
	Estimate for the ECOSAR class: Esters (Phosphinates) ChV 0.054* mg/L	ECOSAR v1.11	QSAR estimate *The toxicity values was estimated through the application of acute-to-chronic ratios

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
		Fish ChV 0.027 mg/L	PBT profiler	QSAR estimate
Daphnid NOEC (Freshwater)		No data located.		
		Estimate for the ECOSAR class: Esters (Phosphinates) ChV 0.051* mg/L	ECOSAR v1.11	QSAR estimate *The toxicity values was estimated through the application of acute-to-chronic ratios
Green Algae NOEC		Test with *Desmodesmus subspicatus* 72 h, EC10 (growth rate) 4.2 mg/L (nominal concentration)	REACH registration data	Reliability 1 OECD Guideline 201
		Aquatic Chronic 3 (H412: Harmful to aquatic life with long-lasting effects)	C&L inventory	Notified classification
Transport		Results of Level III fugacity modelling indicate that at equilibrium the substance will be found almost exclusively in soil (83%) and water (16%), while a small fraction will be in sediment. In the atmosphere, the substance is expected to be present only associated with water aerosols and removal from air is therefore by wet deposition.		
	Henry's Law Constant (atm-m³/mole)	No data located.		
	Sediment/Soil Adsorption/Desorption – K_d/K_{oc}	No data located.		
	Level III Fugacity Model	Media — Percent in each medium Water 16% Soil 83% Sediment 1% Air 0%	PBT profiler	
Persistence		**High:** A half-life was not determined in the OECD ready biodegradability screening test. At the end of the test (28d), only 19% of the test substance was degraded. Persistence is scored as "High" based on an estimated half-life of 140 days in sediment.		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
Water	Aerobic Biodegradation	Activated sludge from a biologic sewage treatment plant was used inoculum (concentration in the test 25.0 mg dry matter/L). The test was left running for 28 days. The following data were determined for the test item KCCS DOB11: 10-day-window: day 11 – 21 degradation at the end of 10-day-window: 16 % degradation at the end of the test: 19 % pass level following guideline: 60% at the end of 10-day-window. Therefore, regardless of the 10-day-window, KCCS DOB11 is not biodegradable following OECD 301B/EU C.4-C.	REACH registration data	Reliability 1 OECD Guideline 301 B
	Volatilization Half-life for Model River	No data located.		
	Volatilization Half-life for Model Lake	No data located.		
Soil	Aerobic Biodegradation	No data located.		
	Anaerobic Biodegradation	No data located.		
	Soil Biodegradation with Product Identification	No data located.		
	Sediment/Water Biodegradation	No data located.		
		No data located.		

6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide/CAS No. 848820-98-4/EC No. 805-659-5				
Property/Endpoint		**Data**	**Reference**	**Comments**
Other	Biotic degradation.	No data located.		
Air	Atmospheric Half-life	No data located.		
Reactivity	Photolysis	No data located.		
	Hydrolysis	No data located.		
Environmental Half-life		Media / Half-life (d) Water 15 Soil 30 Sediment 140 Air 1.3	PBT profiler	
Bioaccumulation		**LOW:** Based on measured log Kow of 3.32.		
	Fish BCF	No data located.		
	Other BCF	80	PBT profiler	QSAR estimate
	BAF	No data located.		
	Metabolism in Fish	No data located.		
Environmental biomonitoring				
Ecological Biomonitoring		No data located.		
Human Biomonitoring		No data located.		

ECOSAR/EPI (EPIWIN/EPISUITE) Estimations Programs Interface for Windows, Version 1.11. U.S. Environmental Protection Agency: Washington D.C. http://www2.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model, Input values: CAS No.: 848820-98-4; Name: 6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide; SMILES: O=C(OCCCC)CCP2(=O)Oc3ccccc3c1ccccc12; Water solubility: 176.1; Log Kow: 3.323.

Metadynea, 2014: DOB11, Technical Data Sheet. November 2014.

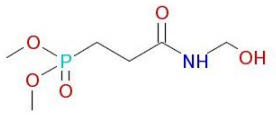
PBTprofiler.net: US EPA PBT Profiler, Model tool available at http://www.pbtprofiler.net/, Input values: CAS No.: 848820-98-4, Name: 6H-Dibenz[c,e][1,2]oxaphosphorin-6-propanoic acid, butyl ester, 6-oxide, SMILES: O=C(OCCCC)CCP2(=O)Oc3ccccc3c1ccccc12.

REACH registration data: http://echa.europa.eu/da/information-on-chemicals/registered-substances using CAS No. 848820-98-4 as search term.

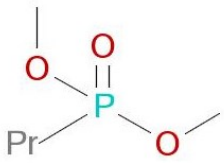
Appendix 10 Technical description of other phosphorous flame retardants

A10.1. Organophosphorous compounds

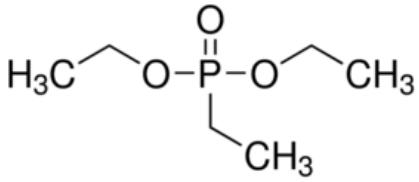
Dimethyl {3-[(hydroxymethyl)amino]-3-oxopropyl}phosphonate, CAS No. 20120-33-6

CAS No	20120-33-6
EC No	243-528-9
Chemical name	Dimethyl {3-[(hydroxymethyl)amino]-3-oxopropyl}phosphonate
Structural formula	 Registration
General formula	C6H14NO5P
Phosphorous content	12% (min) (Everfos CP)
Abbreviation, synonyms	N-Hydroxymethyl-3-dimethylphosphonopropionamide
FR products and manufacturers	Everfors CP (Everkem)
Registered tonnage, t/year	100 – 1,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Cotton textile
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	Alternative to decaBDE for natural cellulose fibres such as cotton, wool, rayon, and linen (Illinois EPA, 2007).
Halogen-containing flame retardants for the same application (examples)	

Dimethyl propyl phosphonate, CAS No. 18755-43-6

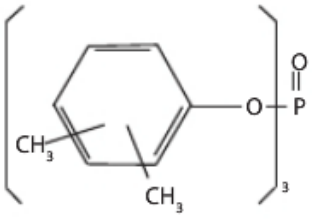
CAS No	18755-43-6		
EC No	242-555-3		
Chemical name	Dimethyl propyl phosphonate		
Structural formula	 Registration		
General formula	C5H13O3P		
Phosphorous content	20.3 % (Levagard DMPP)		
Abbreviation, synonyms	DMPP		
FR products and manufacturers	Levagard DMPP (Lanxess)		
Registered tonnage, t/year	100 – 1,00		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Foams	PUR rigid foams	Applicable
	Textile/Paint/Adhesives	Paints	Applicable
	Thermosets	Unsaturated polyesters	Applicable
		Epoxy resins	Applicable
Other information on substrate	-		
End applications	-		
Reactive/additive	-		
Health env. profiles	-		
Availability	-		
Flame retardancy	-		
Halogen-containing flame retardants for the same application (examples)	Mainly marketed as alternative to dimethyl methylphosphonate not as alternative to halogenated flame retardants		

Diethyl ethylphosphonate, CAS No. 78-38-6

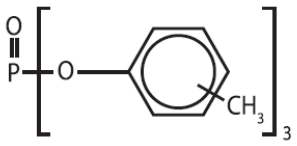
CAS No	78-38-6		
EC No	201-111-9		
Chemical name	Diethyl ethylphosphonate		
Structural formula	 Sigma Aldrich Homepage		
General formula	C6H15O3P		
Phosphorous content	19 % (Aflammit® PLF 822)		
Abbreviation, synonyms			
FR products and manufacturers	Aflammit® PLF 822 (THOR)		
Registered tonnage, t/year	Preregistered		
Pinfa Product Selector	Group: Foams	Substrate: PUR rigid foam	Applicability: applicable
Other information on substrate	"Low viscosity FR for use in rigid PUR and PIR foams. Good compatibility and FR performance at low dosage in epoxy and unsaturated polyesters" (THOR)		
End applications			
Reactive/additive			
Health env. profiles			
Availability			
Flame retardancy			
Halogen-containing flame retardants for the same application (examples)			

A10.2. Organophosphates (phosphate esters) – Aryl phosphates

Trixylyl phosphate, CAS No. 25155-23-1

CAS No	25155-23-1
EC No	246-677-8
Chemical name	Trixylyl phosphate
Structural formula	 Everkem product brochure
General formula	C24H27O4P
Phosphorous content	7.8% (EVERFOS TXP)
Abbreviation, synonyms	TXP
FR products and manufacturers	EVERFOS TXP (Everkem)
Registered tonnage, t/year	100-1,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	EPDM, PVC, PC/ABS (alloys), rigid and flexible polyurethane, phenolics resin, Coating (paint), textile (back coating), adhesive
End applications	
Reactive/additive	
Health env. profiles	Has a harmonised classification according to the CLP regulation as reprotoxic (Repr. 1B) and has consequently not been selected for screening.
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Tricresyl phosphate and trixylenyl phosphate mixture, CAS No. 1330-78-5, 78-32-0, 78-30-8 and 25155-23-1

CAS No	1330-78-5, 78-32-0, 78-30-8 and 25155-23-1
EC No	215-548-8
Chemical name	Tri(m,p-cresyl) phosphate mixture
Structural formula	 Lindol SDS from ICL-IP Europe
General formula	N.a.
Phosphorous content	8.4 (Lindol & Lindol XP Plus)
Abbreviation, synonyms	Tri(m,p-cresyl) phosphate mixture
FR products and manufacturers	Lindol & Lindol XP Plus (ICL-IP Europe)
Registered tonnage, t/year	CAS No. 1330-78-5: 1,000-10,000 CAS No. 25155-23-1: 100-1,000 CAS No. 78-32-0 and 78-30-8: preregistered
Pinfa Product Selector	Product not identified in PPS
Other information on substrate	PVC flexible, Cellulosic Plastic Composite
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Proprietary aromatic phosphate

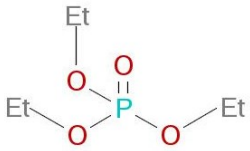
CAS No	Proprietary
EC No	-
Chemical name	Proprietary, aromatic phosphate, solid powder
Structural formula	N.a.
General formula	N.a.
Phosphorous content	10.5% (Fyrolflex Sol-DP)
Abbreviation, synonyms	
FR products and manufacturers	Fyrolflex DP (ICL-IP Europe)
Registered tonnage, t/year	
Pinfa Product Selector	Not identified in PSS
Other information on substrate	HIPS/PPO, PC/PC ABS
End applications	
Reactive/additive	Reactive
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Proprietary halogen-free phosphorous ester

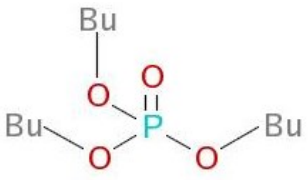
CAS No	Proprietary
EC No	-
Chemical name	Proprietary halogen-free phosphorus ester
Structural formula	N.a.
General formula	N.a.
Phosphorous content	8.5% (Fyrol A710)
Abbreviation, synonyms	
FR products and manufacturers	Fyrol A710 (ICL-IP Europe)
Registered tonnage, t/year	
Pinfa Product Selector	Not identified in PSS
Other information on substrate	Flexible Polyurethane foams
End applications	"recommended for use in the Automotive MVSS302 and furniture California Technical Bulletin 117 flammability tests" (ICL-IP Europe)
Reactive/additive	Additive
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

A10.3. Organophosphates (phosphate esters) – Alkyl phosphates

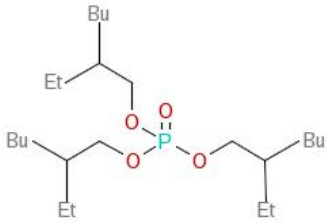
Triethyl phosphate, CAS No. 78-40-0

CAS No	78-40-0		
EC No	201-114-5		
Chemical name	Triethyl phosphate		
Structural formula	 Registration		
General formula	C6H15O4P		
Phosphorous content	17% (Levagard TEP-Z)		
Abbreviation, synonyms	TEP		
FR products and manufacturers	Levagard TEP-Z (Lanxess)		
Registered tonnage, t/year	1,000 – 10,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Foams	PUR rigid foam	Applicable
	Thermosets	Unsaturated polyesters	Applicable
Other information on substrate	PIR / PUR rigid foams and thermosets		
End applications			
Reactive/additive			
Health env. profiles	Not developed		
Availability			
Flame retardancy			
Halogen-containing flame retardants for the same application (examples)			

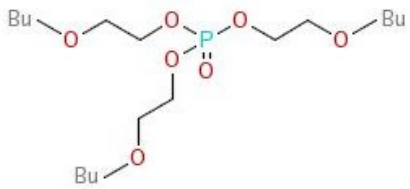
Tributyl phosphate, CAS No. 126-73-8

CAS No	126-73-8
EC No	204-800-2
Chemical name	Tributyl phosphate
Structural formula	 Registration
General formula	C12H27O4P
Phosphorous content	11.7% (Phosflex 4)
Abbreviation, synonyms	TNBO, Tris(butyl) phosphate, Tri-n-butyl phosphate
FR products and manufacturers	Phosflex 4 (ICL-IP Europe)
Registered tonnage, t/year	1,000 – 10,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	PVC flexible, latex/adhesives, cellulosic plastic composite
End applications	
Reactive/additive	Additive
Health env. profiles	Has a harmonised classification according to the CLP Regulations as carcinogenic (Carc. 2) and has consequently not been selected for screening.
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Tris-(2-ethylhexyl) phosphate, CAS No. 78-42-2

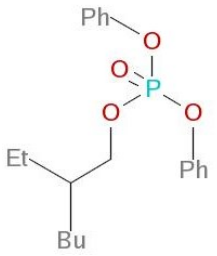
CAS No	78-42-2
EC No	201-116-6
Chemical name	Tris-(2-ethylhexyl) phosphate
Structural formula	 Registration
General formula	C24H51O4P
Phosphorous content	
Abbreviation, synonyms	TEHP
FR products and manufacturers	Disflamoll TOF (Lanxess)
Registered tonnage, t/year	1,000 – 10,000
Pinfa Product Selector	Not included in the Product Selector
Other information on substrate	Many types of polymers including PVC flexible, PUR, NBR, SBR and EPDM.
End applications	
Reactive/additive	Additive
Health env. profiles	Profile not developed
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Tris(2-butoxyethyl)phosphate, CAS No. 78-51-3

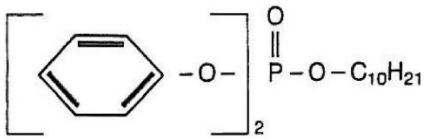
CAS No	78-51-3
EC No	201-114-5
Chemical name	Tris(2-butoxyethyl) phosphate
Structural formula	 Registration
General formula	C18H39O7P
Phosphorous content	7.8% (Phosflex T-BEP)
Abbreviation, synonyms	TBOEP; Ethanol, 2-butoxy-, 1,1′,1″-phosphate; Ethanol,2-butoxy-, phosphate (3:1)
FR products and manufacturers	Phosflex T-BEP (ICL-IP Europe)
Registered tonnage, t/year	1,000 – 10,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Rubbers/elastomers, latex/adhesives
End applications	
Reactive/additive	
Health env. profiles	Profile not developed
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

A10.4. Organophosphates (phosphate esters) – Aryl alkyl phosphates

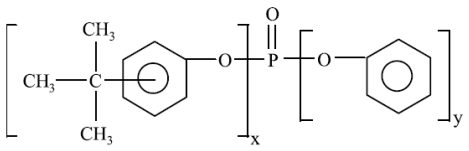
Diphenyl (2-ethylhexyl)phosphate, CAS No. 1241-94-7

CAS No	1241-94-7		
EC No	214-987-2		
Chemical name	Diphenyl (2-ethylhexyl) phosphate		
Structural formula	 Registration		
General formula	$C_{20}H_{27}O_4P$		
Phosphorous content	8.5% (Phosflex 362) 8.6% (Disflamoll DPO)		
Abbreviation, synonyms	DPO		
FR products and manufacturers	Disflamoll DPO (Lanxess) Phosflex 362 (ICL-IP Europe)		
Registered tonnage, t/year	1,000 – 10,000		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Foams	Rubbers/elastomers	Applicable
		PVC/nitrile foam	Applicable
		Paints	Applicable
		PVC flexible	Applicable
Other information on substrate	PVC, thermoplastic polyurethane, nitrile butadiene rubber, cellulose nitrate, cellulose acetate		
End applications			
Reactive/additive			
Health env. profiles	Profile not developed		
Availability			
Flame retardancy			
Halogen-containing flame retardants for the same application (examples)	Non-halogen flame retardants are the main FRs for PVC		

Isodecyl diphenyl phosphate, CAS No. 29761-21-5

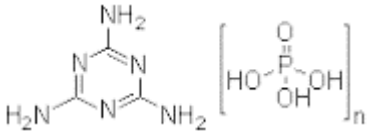
CAS No	29761-21-5
EC No	249-828-6
Chemical name	Isodecyl diphenyl phosphate
Structural formula	 Registration
General formula	C22H31O4P
Phosphorous content	7.9% (Phosflex 390)
Abbreviation, synonyms	8-methylnonyl diphenyl phosphate
FR products and manufacturers	Phosflex 390 (ICL-IP Europe)
Registered tonnage, t/year	1,000 – 10,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	PVC flexible
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	Non-halogenated FRs are the main FRs for flexible PVC

t-butylated triphenyl phosphate mixture, CAS No. 56803-37-3, 65652-41-7, 78-33-1 and 115-86-6

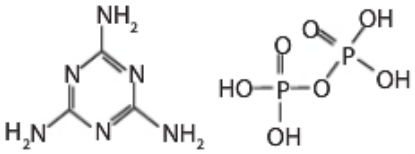
CAS No	56803-37-3, 65652-41-7, 78-33-1 and 115-86-6
EC No	260-391-0, 265-859-8, 201-106-1, and 204-112-2
Chemical name	t-butylated triphenyl phosphate mixture
Structural formula	 x + y = 3 x = 0-3 Phosflex 71B datasheet
General formula	
Phosphorous content	8.5% (Phosflex 71B)
Abbreviation, synonyms	
FR products and manufacturers	Phosflex 71B (ICL-IP Europe)
Registered tonnage, t/year	Substances are preregistered individually, except 115-86-6: 1,000 – 10,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	HIPS/PPO, PC/PC ABS, flexible PVC
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

A10.5. Melamine-derived and other organic phosphates (not being esters)

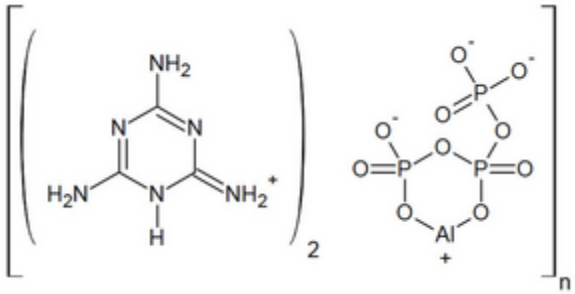
Melamine polyphosphate, CAS No. 218768-84-4

CAS No	218768-84-4		
EC No	*606-855-1		
Chemical name	Melamine polyphosphate		
Structural formula	 Lassen et al., 2006		
General formula	Not available		
Phosphorous content	Not available		
Abbreviation, synonyms	Melapur M 200, Melapur 200, MPP		
FR products and manufacturers	Melapur® 200 range (BASF) BUDIT 3141 (Budenheim) AFLAMMIT® PMN 200 (THOR)		
Registered tonnage, t/year	Pre-registered		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	PET	Applicable
		PBT	Applicable
		Polyamide (PA)	Applicable
		Polypropylene (PP)	Applicable
		HIPS/PPO	Applicable
	Textiles/Paints/Adhesives	Intumescent Coatings	Applicable
	Thermosets	Epoxy Resins	Applicable
		Phenolic Resins	Applicable
		Unsaturated polyesters	Applicable
		Acrylic resins	Applicable
Other information on substrate	-		
End applications	Construction EEE		
Reactive/additive	Additive		
Health env. profiles	Modified profile of the substance with nearly similar structure, CAS No. 15541-60-3, is presented above.		
Availability			
Flame retardancy	Vo-grade glass reinforced PA66 can be obtained with 26% melamine polyphosphate (Lassen et al., 2006) Melamine polyphosphate is mostly used in combination with other flame retardants, such as metal phosphinates, metal hydroxides and phosphates (Rakotamala et al., 2010)		
Halogen-containing flame retardants for the same application (examples)			

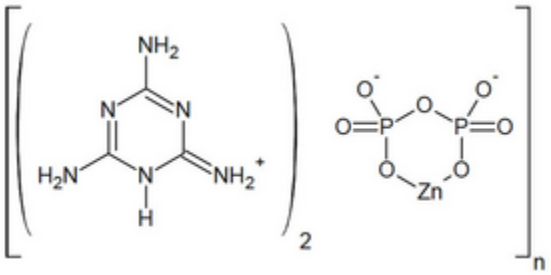
Melamine polyphosphate, CAS No. 20208-95-1

CAS No	20208-95-1
EC No	243-601-5
Chemical name	Melamine polyphosphate (Everkem)
Structural formula	 Everkem product catalogue
General formula	C3H6N6(H3PO4)n (Everkem)
Phosphorous content	>31%
Abbreviation, synonyms	1,3,5-triazine-2,4,6-triamine monophosphate (pre-registration)
FR products and manufacturers	EVERFLAM MPP-1 (Everkem)
Registered tonnage, t/year	Pre-registered
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Polyester, PA
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

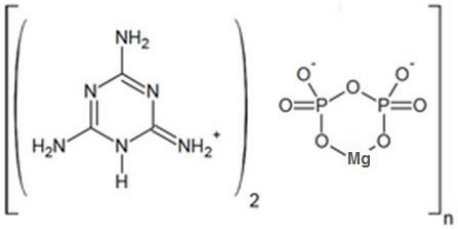
Melamine-poly(aluminium phosphate), CAS No. 1271168-40-1

CAS No	1271168-40-1		
EC No	Not available		
Chemical name	Melamine-poly(aluminium phosphate)		
Structural formula	 Safire presentation		
General formula	Not available		
Phosphorous content	17% (Safire® 200)		
Abbreviation, synonyms			
FR products and manufacturers	Safire® 200 (Floridienne Chimie s.a. (patent belongs to Catena additives)		
Registered tonnage, t/year	Neither registered nor Pre-registered		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	PET	Applicable
		PBT	Applicable
		Polyamide (PA)	Applicable
		Polypropylene (PP)	Applicable
		HIPS/PPO	Applicable
	Textiles/Paints/Adhesives	Intumescent Coatings	Applicable
	Thermosets	Epoxy Resins	Applicable
		Phenolic Resins	Applicable
		Unsaturated polyesters	Applicable
		Acrylic resins	Applicable
Other information on substrate	PA, Nylon, PBT, PE, PP, PS, HIPS, PPE		
End applications	Automotive/ Transportation, Electrical component, Cables, Glass fibers		
Reactive/additive			
Health env. profiles			
Availability			
Flame retardancy			
Halogen-containing flame retardants for the same application (examples)			

Melamine-poly(zinc phosphate), CAS No. 1271172-98-5

CAS No	1271172-98-5		
EC No	Not available		
Chemical name	Melamine-poly(zinc phosphate)		
Structural formula	 Safire presentation		
General formula	Not available		
Phosphorous content	14% (Safire® 400)		
Abbreviation, synonyms			
FR products and manufacturers	Safire ®400 (Floridienne Chimie s.a. (patent belongs to Catena additives)		
Registered tonnage, t/year	Neither registered nor Pre-registered		
Pinfa Product Selector	Group:	Substrate:	Applicability:
	Solid Thermoplastics	PET	Applicable
		PBT	Applicable
		Polyamide (PA)	Applicable
		Polypropylene (PP)	Applicable
		HIPS/PPO	Applicable
	Textiles/Paints/Adhesives	Intumescent Coatings	Applicable
	Thermosets	Epoxy Resins	Applicable
		Phenolic Resins	Applicable
		Unsaturated polyesters	Applicable
		Acrylic resins	Applicable
Other information on substrate	EVA, PA, Nylon, PBT, PE, PUR, PVC flexible, TPE and TPV		
End applications	Automotive/ Transportation, Buildings & construction, Electrical components, Cables, Glass fibers, Compoundings.		
Reactive/additive			
Health env. profiles			
Availability			
Flame retardancy			
Halogen-containing flame retardants for the same application (examples)			

Melamine-poly(magnesium phosphate), CAS No. Not identified

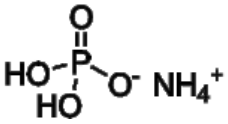
CAS No	Not identified
EC No	Not identified
Chemical name	Melamine-poly(magnesium phosphate)
Structural formula	 Safire presentation
General formula	Not available
Phosphorous content	17.6% (Safire® 600)
Abbreviation, synonyms	
FR products and manufacturers	Safire® 600 (Floridienne Chimie s.a. (patent belongs to Catena additives)
Registered tonnage, t/year	Neither registered nor Pre-registered
Pinfa Product Selector	Not identified in PPS
Other information on substrate	PBT PA, Nylon
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

1,3,5-Triazine-2,4,6-triaminephosphate, CAS No. 94031-26-2

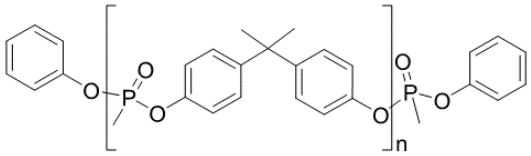
CAS No	94031-26-2
EC No	Not available
Chemical name	1,3,5-Triazine-2,4,6-triaminephosphate
Structural formula	Not available
General formula	Not available
Phosphorous content	16 – 18% (PPP111)
Abbreviation, synonyms	Flame retardant P
FR products and manufacturers	PPP111 (Metadynea Austria GmbH)
Registered tonnage, t/year	Neither registered nor Pre-registered
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Intumescent flame retardant systems
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

A10.6. Inorganic phosphorous compounds

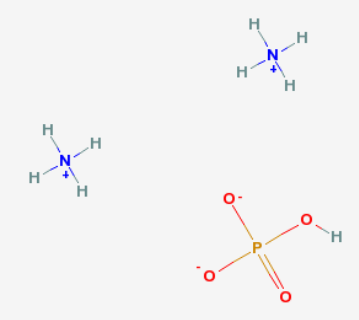
Monoammonium phosphate, CAS No. 7722-76-1

CAS No	7722-76-1
EC No	231-764-5
Chemical name	Monoammonium phosphate
Structural formula	 Registration
General formula	H3N.H3O4P
Phosphorous content	75-85% (PHOS-CHEK® MVP-F (also contains diammonium phosphate)) 8-12% (PHOS-CHEK® MVP-Fx (also contains dinoammonium phosphate))
Abbreviation, synonyms	Ammonium dihydrogenorthophosphate, ammonium phosphate
FR products and manufacturers	PHOS-CHEK® MVP-F (also contains diammonium phosphate), PHOS-CHEK® MVP-Fx (also contains diammonium phosphate) (BK Giulinibk-giulini GmbH)
Registered tonnage, t/year	1,000,000 - 10,000,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	-
End applications	Wildfire control
Reactive/additive	-
Health env. profiles	No profile developed
Availability	Widely avaialble for flame retardancy and other applications
Flame retardancy	-
Halogen-containing flame retardants for the same application (examples)	Wildfire control is not a significant

Polyphosphonate, CAS No. 68664-06-2

CAS No	68664-06-2		
EC No	Not available		
Chemical name	Polyphosphonate (Mn >10,000)		
Structural formula	 US EPA, 2014a		
General formula	C15H16O2(C16H17O3P)n		
Phosphorous content	10.8 wt.%		
Abbreviation, synonyms	FRX 100 (polyphosphonate), Phosphonic acid		
FR products and manufacturers	Nofia HM1100 (FRX Polymers)		
Registered tonnage, t/year	Not reg/pre-reg		
Pinfa Product Selector	Solid Thermoplastics	Themoplastic elastomers	applicable
		PBT	applicable
		PET	applicable
	Textiles/Paints/Adhesives	Other textile fibres	applicable
		Polyester fibres	applicable
	Wire and cables	TPU	applicable
	Solid Thermoplastics	Themoplastic elastomers	applicable
Other information on substrate			
End applications	Fibers: Carpets; Textiles Electronic Equipment and Consumer Electronics: Connectors; Wire & Cable Building and Construction: Transparent sheet products; Transparent blown film Transportation		
Reactive/additive	Additive		
Health env. profiles	Alternatives for the flame retardant decaBDE (US EPA, 2014a)		
Availability	Readily available		
Flame retardancy	Carpets and Textiles: Low Flame Spread; Radiant panel ASTM E-648, NFPA 701, MVSS 302; Connectors: UL94 V0 / 0.8mm Wire and Cable: VW1 (UL1581) Transparent sheet and blown films: E162 - Class A rating; E84 - Class A rating		
Halogen-containing flame retardants for the same application (examples)	DecaBDE		

Diammonium phosphate, CAS No. 7783-28-0

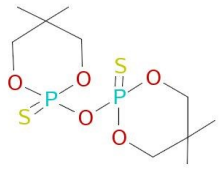
CAS No	7783-28-0
EC No	231-987-8
Chemical name	Diammonium phosphate
Structural formula	 Registration
General formula	H3N.1/2H3O4P
Phosphorous content	8-12% (PHOS-CHEK® MVP-F (also contains monoammonium phosphate)) 75-85% (PHOS-CHEK® MVP-Fx (also contains monoammonium phosphate)) >90% PHOS-CHEK 259-F
Abbreviation, synonyms	Diammonium hydrogenorthophosphate, diammonium hydrogen phosphate
FR products and manufacturers	PHOS-CHEK® MVP-F (also contains monoammonium phosphate), PHOS-CHEK® MVP-Fx (also contains monoammonium phosphate), PHOS-CHEK 259-F, (BK Giulinibk-giulini GmbH)
Registered tonnage, t/year	1,000,000 - 10,000,000
Pinfa Product Selector	Not identified in PPS
Other information on substrate	Wildfire control
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Aluminium phosphates, CAS No. Not identified

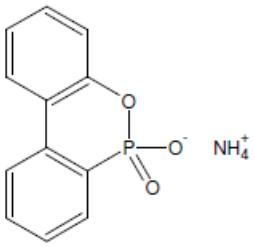
CAS No	Not identified
EC No	Not identified
Chemical name	Aluminium phosphates
Structural formula	Not available
General formula	Not available
Phosphorous content	Not available
Abbreviation, synonyms	
FR products and manufacturers	FR CROS 134 P, FR CROS 134 T (Budenheim)
Registered tonnage, t/year	
Pinfa Product Selector	Not identified in PPS
Other information on substrate	
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

A10.7. Other phosphorous and non-categorised substances

2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulphide, CAS No. 4090-51-1

CAS No	4090-51-1		
EC No	223-829-1		
Chemical name	2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulphide		
Structural formula	 Registration		
General formula	C10H20O5P2S2		
Phosphorous content	Not available		
Abbreviation, synonyms			
FR products and manufacturers	Exolit® 5060 PK (Clariant) Mileflame FR 5060 (MPI Chemie)		
Registered tonnage, t/year	100 – 1,000		
Pinfa Product Selector	Group: Textiles/Paints/Adhesives	Substrate: Viscose	Applicability: Applicable
Other information on substrate	Viscose fibres		
End applications			
Reactive/additive			
Health env. profiles			
Availability			
Flame retardancy			
Halogen-containing flame retardants for the same application (examples)	Viscose fibres is not a significant application of halogenated flame retardants		

Ammonium 6H-dibenzo[c,e][1,2]oxaphosphinin-6-olate 6-oxide,
CAS No. 1402947-09-4

CAS No	1402947-09-4
EC No	Not available
Chemical name	Ammonium 6H-dibenzo[c,e][1,2]oxaphosphinin-6-olate 6-oxide
Structural formula	 Technical Data Sheet for DXA 12
General formula	
Phosphorous content	12.0 – 12.5 % (DXA 12)
Abbreviation, synonyms	
FR products and manufacturers	DXA 12 (Metadynea Austria GmbH)
Registered tonnage, t/year	Neither registered nor Pre-registered.
Pinfa Product Selector	Not identified in PPS
Other information on substrate	
End applications	
Reactive/additive	
Health env. profiles	
Availability	
Flame retardancy	
Halogen-containing flame retardants for the same application (examples)	

Environmental and health screening profiles of phosphorous flame retardants
This is a survey that identifies phosphorous flame retardants and develops screening level substance hazard profiles, to be used for substitution consideration in a European REACH context by companies using flame retardants. The screening hazard profiles have been prepared based on a modified version of a method for hazard assessment of chemicals known as GreenScreen®. The GreenScreen® method was developed in the USA for the US EPA "Design for the Environment" (DfE) programme and consists of a hazard profiling part and a "benchmarking" part aimed to assess the relevance of a substance for consideration in a substitution context. For the purpose of the current project, the method has been reviewed and adapted as appropriate for use in a European regulatory context.

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