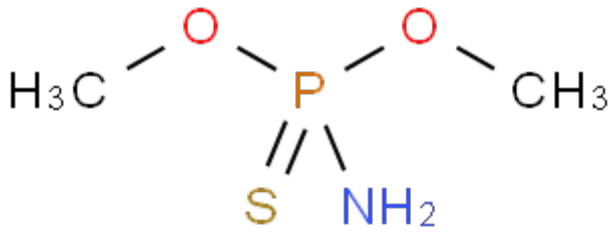
Miljøministeriet
Miljøstyrelsen

Fastsættelse af kvalitetskriterier for vandmiljøet

O,O-dimethyl fosforamidothioat (DMPAT)

CAS nr. 17321-47-0



Vandkvalitetskriterium	$VKK_{ferskvand}$	Ikke muligt at udlede
Vandkvalitetskriterium	$VKK_{saltvand}$	Ikke muligt at udlede
Korttidsvandkvalitetskriterium	$KVKK_{ferskvand}$	Ikke muligt at udlede
Korttidsvandkvalitetskriterium	$KVKK_{saltvand}$	Ikke muligt at udlede
Sedimentkvalitetskriterium	$SKK_{ferskvand}$	Ikke udledt
Sedimentkvalitetskriterium	$SKK_{saltvand}$	Ikke udledt
Biota-kvalitetskriterium, sekundær forgiftning	$BKK_{sek.forgiftn.}$	Ikke udledt
Biota-kvalitetskriterium, human konsum	HKK	Ikke udledt

5. december 2023

Indholdsfortegnelse

Forord

Et kvalitetskriterium i vandmiljøet er det højeste koncentrationsniveau, ved hvilket der skønnes, ikke at forekomme uacceptable negative effekter på vandøkosystemer.

Miljøstyrelsen (MST) udarbejder kvalitetskriterier for kemikalier i vandsøjlen, i sediment, i dyr og planter (biota) og for human konsum.

Miljøstyrelsen bruger kvalitetskriterierne som det faglige grundlag til at kunne fastsætte miljøkvalitetskrav, hvorved der forstås den endelige koncentration af et bestemt forurenende stof i vand, sediment eller biota, som ikke må overskrides af hensyn til beskyttelsen af miljøet og menneskers sundhed.

Metodikken, der anvendes til udarbejdelse af miljøkvalitetskrav er harmoniseret i EU og baserer sig på vandrammedirektivet (EU, 2000), EU's vejledning til fastsættelse af kvalitetskriterier i vandmiljøet (EU, 2018) og Miljøstyrelsens vejledning til fastsættelse af vandkvalitetskriterier (MST, 2004). Metodikken er endvidere i overensstemmelse med EU's vejledning til risikovurdering under REACH forordningen (EU, 2008).

Den seneste litteratursøgning er foretaget september 2023.

English Summary and conclusions

Derivation of environmental quality standards (EQS) for the aquatic environment is following the EU Guidance Document No. 27. Technical Guidance Document for Deriving Environmental Quality Standards (TGD) (EU, 2018).

O,O-phosphoramidothioate (DMPAT) is an intermediate in production of other chemicals, e.g. organophosphorus insecticides.

QS for freshwater and saltwater

Short-term ecotoxicity data have been available for the two marine species: *Skeletonema costatum* (algae) and *Acartia tonsa* (crustacean). Long-term ecotoxicity data have been available for one marine species: *Skeletonema costatum* (algae). Furthermore, data have been supported by QSAR data for freshwater organisms from the Danish (Q)SAR Model and the NORMAN Database. Based on the available data, it is however not possible to conclude which trophic level is most sensitive to DMPAT.

The toxicity data base set (fish, invertebrates and algea) is not complete according to TGD (EU, 2018), since there are no data on fish. It is therefore not possible to derive neither an annual average quality standard (AA-QS) nor a maximum acceptable concentration (MAC-QS).

QS for sediment

According to TGD (EU, 2018) it is relevant to derive a QS for sediment (QS_{sed}) for a substance if log K_{ow} or log K_{oc} is ≥ 3 or if there is other evidence for accumulation in sediments or high toxicity to benthic organsims. For DMPAT, both log K_{OW} and log K_{OC} are estimated to be below 3 (0.2 and >1.1 respectively), and there are no other evidence for accumulation in sediments. The criteria for deriving a QS for sediment is therefore not fulfilled.

QS for secondary poisoning

According to TGD (EU, 2018) it is relevant to derive a QS for secondary poisoning ($QS_{sec.\ pois.}$) if BCF (BAF) ≥ 100. DMPAT has a low estimated log K_{OW} (0.2) and an estimated bioconcentration factor (BCF) below 100 (1.1-3.2 l/kg), indicating a low potential for bioaccumulation and accumulation in the food chain. The criteria for deriving a QS for secondary poisoning is therefore not fulfilled.

QS for human health

According to TGD (EU, 2018), a QS for human consumption of fishery products ($QS_{human\ health}$) is relevant if the substance has relevant human hazard properties. DMPAT poses no known hazards for carcinogenic, mutagenic or reprotoxic effects, or known risk of irriversibel effects. DMPAT is furthermore expected to have a low potential for bioaccumulation. The criteria for deriving a QS for human health is therefore not fulfilled.

In conclusion, the following EQS for the aquatic environment have been derived for DMPAT:

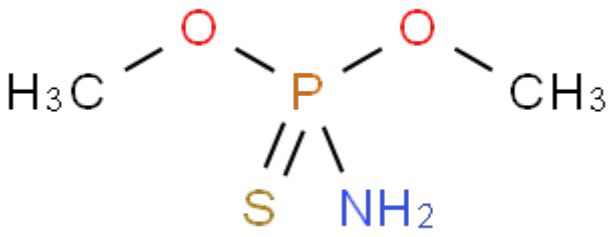
$AA\text{-}QS_{freshwater}$	= not possible to derive
$AA\text{-}QS_{saltwater}$	= not possible to derive
$MAC\text{-}QS_{freshwater}$	= not possible to derive
$MAC\text{-}QS_{saltwater}$	= not possible to derive
$QS_{sediment,\ freshwater}$	= not determined
$QS_{sediment,\ saltwater}$	= not determined
$QS_{biota,\ secondary\ poisoning}$	= not determined
$QS_{biota,\ human\ health}$	= not determined

1 Indledning

O,O-dimethyl fosforamidothioat (DMPAT) er et syntetisk stof, som anvendes industrielt ved fremstilling af andre stoffer, f.eks. organofosfat-insekticider som acephat og methamidophos (Zhou et al., 2022).

Identiteten af DMPAT fremgår af tabel 1.1.

Tabel 1.1. Identitet af DMPAT

IUPAC navn	[amino(methoxy)phosphinothioyl]oxymethane
Andre navne	O,O-dimethyl thiophosphoramidate O,O-dimethyl phosphoramidothioate
Strukturformel	
CAS nr.	17321-47-0
EINECS nr.	241-342-2
Kemisk formel	$C_2H_8NO_2PS$
SMILES	COP(N)(=S)OC
Harmoniseret klassificering	Ingen harmoniseret klassificering
Selvklassificering	Ingen selvklassificering

2 Fysisk kemiske egenskaber

De fysisk kemiske egenskaber for DMPAT fremgår af tabel 2.1.

Grundet få eksperimentelle data, er QSAR-modeller anvendt til at estimere fysisk kemiske egenskaber for DMPAT. Resultaterne fremgår af bilag A (Danish (Q)SAR) og bilag B (CompTox Chemicals Dashboard).

Tabel 2.1. Fysisk kemiske egenskaber for DMPAT

Parameter	**Værdi**	**Reference**
Molekylevægt, M_w ($g \cdot mol^{-1}$)	141,13	Danish (Q)SAR
Smeltepunkt, T_m (ºC)	-63,81 -63,8 - 108[a]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Kogepunkt, T_b (ºC)	180,76 162 - 246[a]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Damptryk, P_v (Pa)	124 0,02013 – 291,98[a,b]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Henry's konstant, H ($Pa \cdot m^3 \cdot mol^{-1}$)	0,3105[a] 0,01723[a,c]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Vandopløselighed, S_w ($g \cdot L^{-1}$)	56,36 - 67,33[a] 26,25 – 162,30[a,d]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Dissociationskonstant, pK_a	Ingen syregruppe fundet 8,43[a]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Octanol/vand fordelingskoefficient, log K_{ow}	0,2[a] -0,768 - 0,203[a]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1
Sediment/vand fordelingskoefficient, normaliseret til organisk karbon, K_{oc} ($L \cdot kg^{-1}$)	8,79 - 11,67[a] 3,02[a]	Danish (Q)SAR CompTox Chemicals Dashboard v2.2.1

[a] Estimeret værdi

[b] Omregnet fra $1{,}51 \cdot 10^{-4}$ – 2,19 mmHg, som er angivet i modellen ($1{,}51 \cdot 10^{-4}$ mmHg · 133,322 Pa/mmHg = 0,02013 Pa; 2,19 mmHg · 133,322 Pa/mmHg = 291,98 Pa)

[c] Omregnet fra $1{,}70 \cdot 10^{-7}$ $atm \cdot m^3 \cdot mol^{-1}$, som er angivet i modellen ($1{,}70 \cdot 10^{-7}$ $atm \cdot m^3 \cdot mol^{-1}$ · 101325 Pa/atm = 0,01723 $Pa \cdot m^3 \cdot mol^{-1}$)

[d] Omregnet fra 0,186-1,15 mol/l, som er angivet i modellen (0,186 mol/L · 141,1292 g/mol = 26,25 g/L; 1,15 mol/L · 141,1292 g/mol = 162,30 g/L)

3 Skæbne i miljøet

Der er søgt efter data for skæbne i miljøet i let tilgængelige oversigtsværker og sammenfattende rapporter suppleret med data fra QSAR-databaser og QSAR-beregninger:

- ECHA-databasen
- US EPA
- CompTox Chemicals Dashboard
- eChemportal
- Søgning i det Kongelige Biblioteks søgetjenester og særsamliger (søgt på stofnavne og CAS nr.)
- Danish (Q)SAR Database

Der blev ikke fundet eksperiementelle data på skæbne i miljøet, og derfor er der suppleret med QSAR fra den danske QSAR database (Danish (Q)SAR Database, 2023), som bl.a. indeholder QSAR fra EPI Suite. Resultaterne fremgår af bilag A.

3.1 Nedbrydelighed

Der foreligger ingen eksperimentel data på nedbrydeligheden af DMPAT. Udfra resultaterne fra Danish (Q)SAR Database (2023) vurderes DMPAT at være ikke let bionedbrydeligt (se bilag A).

3.2 Bioakkumulering

Der er ikke fundet eksperimentelle data for bioakkumulering. DMPAT har en lav estimeret log K_{OW} på 0,2 (se tabel 2.1). Derudover estimeres biokoncentrationsfaktoren (BCF) ved EPI BCFBAF modellerne til 3,162 l/kg vådvægt samt ved BCF Arnot-Gobas inklusiv biotransformering til 1 l/kg vådvægt (Danish (Q)SAR Database, 2023). I CompTox estimeres BCF til 2,63 (estimeret med OPERA 2.6), hvilket er på niveau med de estimerede værdier fra Danish (Q)SAR. Bioakkumuleringspotentialet for DMPAT i akvatiske organismer forventes således at være lavt.

3.3 Naturlig forekomst

Der foreligger ikke oplysninger om, at DMPAT forekommer naturligt.

4 Toksicitetsdata

To forsøgsrapporter med eksperimentelle studier på stoffets toksicitet overfor vandlevende organismer af DMPAT (Winther-Nielsen, 2005 og Bjørnestad, 2005) har været tilgængelige for udarbejdelsen af miljøkvalitetskriterier i nuværende datablad.

Derudover er der søgt data i lettilgængelige oversigtsværker og sammenfattende rapporter:

- ECHA-database
- ECOTOX-databasen
- US EPA
- IRIS
- CompTox Chemicals Dashboard
- cChemportal
- NORMAN Ecotoxicology Database
- EFSA
- Søgning i det Kongelige Biblioteks søgetjenester og særsamlinger (søgt på stofnavne og CAS nr.)

Der er ikke fundet eksperimentelt data for toksiciteten af DMPAT ud over forsøgsrapporterne med økotoksikologisk karakterisering af DMPAT (Winther-Nielsen, 2005 og Bjørnestad, 2005). Derfor er data suppleret med QSAR (Danish (Q)SAR samt informationer fra NORMAN Ecotoxicology Database). QSAR-resultaterne fremgår af bilag A.

Data fra studier er troværdighedsvurderet udfra CRED-metoden (Moermond et al., 2016), hvor studierne tildeles en score fra 1 til 4. Score 1 angiver, at studiet kan anvendes uden forbehold, mens score 2 angiver, at studiet kan anvendes med forbehold, f.eks. at der er tilstrækkelige oplysninger, selvom studiet ikke er udført i henhold til en guideline. Studier, som har tydelige mangler, tildeles en score 3, mens score 4 tildeles studier, hvor det ikke er muligt at vurdere kvaliteten og dermed troværdigheden, f.eks. hvis studiet ikke er tilgængeligt. Estimerede værdier tildeles en score 3, f.eks. QSAR-resultater.

4.1 Toksicitet over for vandlevende organismer

Den akutte toksicitet af DMPAT er testet på to marine arter, repræsenterende to forskellige trofiske niveauer: *Skeletonema costatum* (alge) og *Acartia tonsa* (invertebrat).

Tabel 4.1 Akutte effekter af DMPAT på marine arter

Art	Varighed	Effekt	Værdi mg/l	Reference	Troværdighed (CRED: 1-4)
Alger					
Skeletonema costatum	72 timer	E_rC_{50} (vækshæmning)	80	Winther-Nielsen, 2005	2
Invertebrater					
Acartia tonsa	48 timer	LC_{50}	1771	Bjørnestad, 2005	2

Den akutte toksicitet overfor den marine invertebrat, *Acartia tonsa*, er undersøgt i henhold til ISO standard testguidelinen 14669 (Dansk Standard, 1999). Effektkoncentrationen, LC_{50}, blev beregnet ved probit-analyse til 1771 mg/l (Bjørnestad, 2005).

Den akutte toksicitet overfor den marine alge, *Skeletonema costatum*, er undersøgt i henhold til ISO standard testguidelinen 10253 (Dansk Standard, 2016) samt OECD-vejledning nr. 201 (OECD, 1984). Effektkoncentrationen, E_rC_{50}, blev beregnet med programmet TOXEDO til 80 mg/l (Winther-Nielsen, 2005).

Toksicitetstest på alger er flergenerationstest, da alger gennemgår flere generationer indenfor en kort eksponeringstid (f.eks. 72 timer) (EU, 2018). De kroniske effektkoncentrationer er derfor beregnet på samme datagrundlag som den akutte effektkoncentration for den marine alge, *Skeletonema costatum*. Effektkoncentrationen, ErC_{10}, blev beregnet med programmet TOXEDO til 55 mg/l, og den højeste koncentration unden signifikant effekt, NOEC, blev estimeret ved variansanalyse med Dunnett's procedure til 50 mg/l (Winther-Nielsen, 2005). De kroniske effektkoncentrationer er sammenstillet i tabel 4.2.

Tabel 4.2 Kroniske effekter af DMPAT på marine arter

Art	Varighed	Effekt	Værdi mg/l	Reference	Troværdighed (CRED: 1-4)
Alger					
Skeletonema costatum	72 timer	E_rC_{10} (vækshæmning)	55	Winther-Nielsen, 2005	2
Skeletonema costatum	72 timer	NOEC (vækshæmning)	50	Winther-Nielsen, 2005	2

Der er ikke fundet eksperimentelle toksicitetsdata på ferskvandslevende arter, og derfor er QSAR-modeller anvendt til at estimere toksiciteten af DMPAT overfor ferskvandslevende arter. QSAR-resultaterne fremgår af bilag A (Danish (Q)SAR) og bilag C (NORMAN Database). De estimerede effektkoncentrationer er sammenstillet i tabel 4.3.

Tabel 4.3 Estimerede akutte effekter af DMPAT på ferskvandslevende arter

Art	Varighed	Effekt	Værdi mg/l	Reference	Troværdighed (CRED: 1-4)
Alger					
Grønne alger	96 timer	EC_{50}	129,08	Danish (Q)SAR	3
Selenastrum capricornutum	72 timer	EC_{50}	52,43	NORMAN Database	3
Invertebrater					
Daphnier	48 timer	EC_{50}	0,041	Danish (Q)SAR	3
Daphnia magna	48 timer	EC_{50}	2,90	NORMAN Database	3
Fisk					
Fisk	96 timer	LC_{50}	18,73	Danish (Q)SAR	3
Pimephales promelas	96 timer	LC_{50}	55,69	NORMAN Database	3

Tallene fra Danish (Q)SAR er beregnet med ECOSAR, mens tallene fra NORMAN Database er beregnet med baggrund i Aalizadeh et al. (2017). De estimerede effektkoncentrationer for ferskvandslevende organismer har en lav troværdighed, og derfor anbefales det ikke at anvende de estimerede effektkoncentrationer direkte i udledningen af vandkvalitetskriterier (EU, 2018).

De estimerede akutte effekter af DMPAT på ferskvandslevende arter indikerer at invertebrater er den mest følsomme taksonomiske gruppe, mens tests med marine arter viser at algen *Skeletonema costatum* er mere følsom end invertebraten *Acartia tonsa*. De estimerede akutte effekter på ferskvandsalger er på niveau med de akutte effekter på marine alger.

Da der ikke foreligger data på fisk, vides det ikke om alger eller fisk er den mest følsomme marine gruppe. Samtidig indikerer estimerede værdier at ferskvandslevende invertebrater kan være mere følsomme end marine arter. Det er derfor ikke muligt at vurdere hvilket trofisk niveau, der er det mest følsomme overfor DMPAT.

4.2 Toksicitet over for sedimentlevende organismer

Der er ikke fundet toksicitetsdata overfor sedimentlevende organismer.

4.3 Toksicitet over for pattedyr og fugle

Der er ikke fundet toksicitetsdata overfor pattedyr og fugle.

Danish (Q)SAR angiver en estimeret LD_{50} i rotter på 270 mg/kg/dag og en estimeret LD_{50} i mus på 600 mg/kg/dag (begge værdier er angivet med "moderat kvalitet").

4.4 Toksicitet over for mennesker

Der er ikke fundet toksicitetsdata overfor mennesker.

5 Andre effekter

Der er ikke fundet oplysninger om andre effekter.

6 Udledning af vandkvalitetskriterium

6.1 Vandkvalitetskriterium (VKK)

Der foreligger et enkelt kronisk studie på en marin art, repræsenterende et enkelt trofisk niveau: Alge (*Skeletonema costaum*). Derudover foreligger der akutte toksicitetsdata på to marine arter, repræsenterende to forskellige trofiske niveauer (alge og invertebrat). Basis-datasættet er således ikke opfyldt jf. TGD (EU, 2018), da der mangler data på akut toksicitet for fisk. Det er derfor ikke muligt at udlede et vandkvalitetskriterie for DMPAT.

6.2 Korttidsvandkvalitetskriterium (KVKK)

Der foreligger akutte toksicitetsdata på to marine arter, repræsenterende to forskellige trofiske niveauer: Alge (*Skeletonema costatum*) og invertebrat (*Acartia tonsa*). Basis-datasættet er således ikke opfyldt jf. TGD (EU, 2018), da der mangler data på fisk. Det er derfor ikke muligt at udlede et korttidsvandkvalitetskriterie for DMPAT.

6.3 Kvalitetskriterium for sediment (SKK)

DMPAT forventes at have lavt potentiale for adsorption i jord og sediment (estimeret K_{OC} = 8,8-11,7), og derfor opfylder stoffet ikke kriteriet ($K_{OC} \geq 100$) for udarbejdelse af et sedimentkvalitetskriterium ifølge TGD (EU, 2018).

6.4 Kvalitetskriterium for biota, sekundær forgiftning ($BKK_{sek.\ forgiftn.}$)

DMPAT forventes at have et lavt bioakkumuleringspotentiale (estimeret log K_{OW} = 0,2 og estimeret BCF = 1,1-3,2), og derfor opfylder stoffet ikke kriteriet (BCF ≥ 100 eller log $K_{OW} \geq 3$), for udarbejdelse af et kvalitetskriterium for biota ifølge TGD (EU, 2018).

6.5 Kvalitetskriterium for human konsum af vandlevende organismer (HKK)

DMPAT er ikke klassificeret som kræftfremkaldende, mutagent eller reproduktionstoksisk, og forventes ikke at have potentiale for at bioakkumulere. Derfor opfylder stoffet ikke kriteriet for udarbejdelse af et kvalitetskriterium for human konsum af fisk og skaldyr ifølge TGD (EU, 2018).

6.6 Vandkvalitetskriterium baseret på $BKK_{sek.\ forgiftn.}$ og HKK

Der er ikke udledt biotakvalitetskriterier, og tilbageberegning til en vandkoncentration er derfor ikke relevant.

7 Konklusion

Grundet begrænset datamængde har det ikke været muligt at udlede miljøkvalitetskriterier for DMPAT:

$VKK_{ferskvand}$	Ikke muligt at udlede
$VKK_{saltvand}$	Ikke muligt at udlede
$KVKK_{ferskvand}$	Ikke muligt at udlede
$KVKK_{saltvand}$	Ikke muligt at udlede
$SKK_{ferskvand}$	Ikke udledt
$SKK_{saltvand}$	Ikke udledt
$BKK_{sek.forgiftn.}$	Ikke udledt
HKK	Ikke udledt

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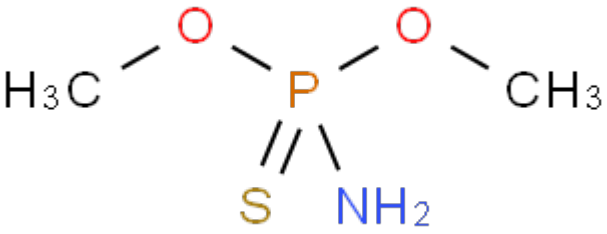
Bilag A: Resultater fra Danish (Q)SAR Model

Danish (Q)SAR Database, http://qsar.food.dtu.dk Date: 27-01-2023

(Q)SAR predicted profile

Structure (as used for QSAR prediction):



SMILES (used for QSAR prediction): COP(N)(=S)OC

ID

Registry Number	17321-47-0	PubChem CID	
REACH EC Number (pre-registration, by 2013)	241-342-2	REACH EC Number (registration, 2019 or 2022)	
REACH registration (2022)		REACH registration cumulated minimum annual tonnage (2022)	
EU CLP Harmonized Classification*		DK-EPA / DTU QSAR-based CLP Advisory Classification	Acute Tox. 4; Aquatic Acute 1
EU Biocide active substances		EU Pesticide active substances	
EU EFSA Botanical substances		US TSCA (Oct. 2021)	Yes
Tox21 (2019)	Yes	ToxCast (Oct. 2021)	
Molecular Formula	C2 H8 N1 O2 P1 S1	Molecular weight (g/mole)	141.13
Chemical Name	O,O-dimethyl thiophosphoramidate		

(Annex VI to CLP up to and including the 9th ATP, and including Nordic Council of Minister SPIN list for group entries)

Melting point, Boiling point and Vapour pressure

Melting Point (deg C)	-63.81	Melting Point Experimental (deg C)	
Boiling Point (deg C)	180.76	Boiling Point Experimental (deg C)	
Vapour Pressure (atm)		Vapour Pressure Experimental (atm)	
Vapour Pressure (mm Hg)	0.93	Vapour Pressure Experimental (mm Hg)	
Vapour Pressure (Pa)	124	Vapour pressure Subcooled Liquid (Pa)	

EPI MPBPVP models

Henry's Law Constant

HLC Bond Method (atm-m3/mole)	7.315E-007	HLC Group Method (atm-m3/mole)	
HLC Via VP/WSol (atm-m3/mole)	3.064E-006	HLC Via VP/WSol (Pa-m3/mole)	0.3105
Henrys Law Const. Exp db (Pa-m3/mole)		Henrys Law Const. Exp db (atm-m3/mole)	

EPI HENRYWIN models

Water Solubility

Water solubility from Kow (mg/L)	56360	Water solubility from Fragments (mg/L)	67327
Water solubility Exp (mg/L)		Water solubility Exp Ref	

EPI WATERNT model

Hydrolysis

Hydrolysis Ka half-life pH 7	Hydrolysis Kb half-life pH 7
Hydrolysis Ka half-life pH 8	Hydrolysis Kb half-life pH 8

EPI HYDROWIN model

pKa

pKa Acid	999
- Standard deviation (±)	0
pKa Base	-999
- Standard deviation (±)	0

ACDLabs model

pKa estimate 999: no acidic moiety found. pKa estimate -999: no basic moiety found.

Partition coefficients

pH	1	4	5	6	7	8	9
LogD	0.42	0.42	0.42	0.42	0.42	0.42	0.42

Minimum LogD in the pH interval 4-9	0.42	Maximum LogD in the pH interval 4-9	0.42

ACDLabs models
LogD: Log octanol-water partition coefficient, which for ionizable compounds varies with the pH-dependent amounts of neutral and ionized species

Log Koa	4.725	Log Kaw	-4.525

EPI KOAWIN models
Koa: octanol-air partition coefficient. Kaw: air-water partition coefficient.

Log Kow	0.2		
Log Kow Exp		Log Kow Exp Ref	

EPI WSKOW model
LogKow: log octanol-water partition coefficient

Kp (m3/ug) Mackay-based	2.66E-008	Kp (m3/ug) Koa-based	1.3E-008
Phi Junge-Pankow-based	9.61E-007	Phi Mackay-based	2.13E-006
Phi Koa-based	1.04E-006		

EPI AEROWIN models
Kp: particle-gas partition coefficient. Phi: fraction of substance sorbed to atmospheric particulates

Koc from MCI (L/kg)	11.67	Log Koc from MCI	1.067
Koc from Kow (L/kg)	8.79	Log Koc from Kow	0.944

EPI KOCWIN models
Koc: soil adsorption coefficient of organic compounds. Kow: octanol-water partition coefficient. MCI: first order Molecular Connectivity Index

Level III Fugacity Environmental Partitioning, emission to air, water and soil

	Air	Water	Soil	Sediment
Mass Amount (%)	0.14	39.3	60.5	0.0912
Half-Life (hr)	1.05	360	720	3240
Emissions (kg/hr)	1000	1000	1000	0

EPI Level III Fugacity Model

Persistence time (hr)	375
Persistence time (days)	15.625

EPI Level III Fugacity Model

Level III Fugacity Environmental Partitioning, emission only to water

	Air	Water	Soil	Sediment
Mass Amount (%)	0.00111	99.8	0.00247	0.232
Half-Life (hr)	1.05	360	720	3240
Emissions (kg/hr)	0	1000	0	0

EPI Level III Fugacity Model

Persistence time (hr)	342
Persistence time (days)	14.25

EPI Level III Fugacity Model

Sewage Treatment Plant (STP) overall chemical mass balance using 10,000 hr

	Total removal	Biodegradation	Sludge Adsorption	Volatilization
(%)	1.89	0.09	1.76	0.04

EPI STPWIN model

Atmospheric oxidation (25 deg C)

	OH	Ozone
Half-Life (d)	0.04521	0
Half-Life (hr)	0.543	
Overall Rate Const. (OH: E-12 cm3/molecule-sec and OZ: E-17 cm3/molecule-sec)	236.576	

EPI AOPWIN models

Biodegradation

Biowin1 (linear model) Probability of Rapid Biodegradation	0.6804
Biowin2 (non-linear model) Probability of Rapid Biodegradation	0.732
Biowin3 Expert Survey Ultimate Biodegradation	2.8873
Biowin3 Expert Survey Ultimate Timeframe	weeks
Biowin4 Expert Survey Primary Biodegradation	3.6441
Biowin4 Exp. Survey Primary Timeframe	days-weeks
Biowin5 (MITI linear model) Biodegradation Probability	0.2931
Biowin6 (MITI non-linear model) Biodegradation Probability	0.181
Biowin7 (Anaerobic Linear) Biodegradation Probability	0.6769
Petroleum Hydrocarbon Biodegradation Half-Life (days)	

EPI BIOWIN models

SkinBiowin1 and Biowin2: ≥0.5: "Rapid" <0.5: "Slow"
Biowin3 and Biowin4: 5 ~ hours; 4 ~ days; 3 ~ weeks; 2 ~ months; 1 ~ years.
Biowin5 and Biowin6: ≥0.5: "Readily", <0.5: "Not readily".
Biowin7: ≥0.5: "Fast", <0.5: "Slow"

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Not Ready Biodegradability (POS=Not Ready)		POS_OUT	POS_OUT	INC_OUT	POS_IN

DTU-developed models

Bioaccumulation

BCF (L/kg wet-wt)	3.162
Log BCF (L/kg wet-wt)	0.5
Whole Body Primary Biotransformation Fish Half-Life (days)	0.04482
BCF Arnot-Gobas (upper trophic) Including Biotransformation (L/kg wet-wt)	1
BCF Arnot-Gobas (upper trophic) Zero Biotransformation (L/kg wet-wt)	1.061
BAF Arnot-Gobas (upper trophic) Including Biotransformation (L/kg wet-wt)	1
BAF Arnot-Gobas (upper trophic) Zero Biotransformation (L/kg wet-wt)	1.063

EPI BCFBAF models
BCF: Bioconcentration factor, BAF: Bioaccumulation factor

Aquatic toxicity

Exp	Battery	Leadscope	SciQSAR
Fathead minnow 96h LC50 (mg/L)		82.47064	303.4725
Domain	OUT	OUT	OUT
Daphnia magna 48h EC50 (mg/L)		16.56339	1.240793
Domain	OUT	OUT	OUT
Pseudokirchneriella s. 72h EC50 (mg/L)		66.57166	72.94898
Domain	OUT	OUT	OUT

DTU-developed models

	Fish 96h	Daphnid 48h	Green Algae 96h
LC50 (Fish) or EC50 (Daphnid and Algae) for Most Toxic Class (mg/L)	18.726	0.041	129.077
Max. Log Kow for Most Toxic Class	5	5	6.4
Most Toxic Class	Esters, Monothiophosphates	Esters, Monothiophosphates	Esters, Monothiophosphates
Note			

EPI ECOSAR models
ECOSAR Classes: Esters, Monothiophosphates

Oral absorption

Lipinski's Rule-of-five score (bioavailability)	0
Absorption from gastrointestinal tract for 1 mg dose (%)	50
Absorption from gastrointestinal tract for 1000 mg dose (%)	50

Leadscope model on Lipinski's Rule-of-five. Equation from literature on GI abs.
Lipinski scores of 0 or 1: The substance may be bioavailable. Lipinski scores of 2, 3 or 4: The substance may not be bioavailable.

Skin absorption

Dermal absorption (mg/cm2/event)	0.0329

EPI DERMWIN model

Brain/blood Distribution

Log brain/blood partition coefficient	-0.3408

Equation from literature
Partitioning between the two tissues at equilibrium. >1: high, >0 to <1: medium, >-1 to <0, fair, <-1: low.

Metabolism

Exp	Battery	CASE Ultra	Leadscope	SciQSAR
CYP2C9 substrates (Human clinical data)	NEG_OUT	INC_OUT	NEG_OUT	NEG_IN
CYP2D6 substrates (Human clinical data)	NEG_OUT	INC_OUT	NEG_OUT	NEG_IN

DTU-developed models

Acute toxicity in Rodents

	LD50 (mg/kg/d)	Reliability Index
Rat Oral	270	0.61
Rat Intraperitoneal	280	0.28
Mouse Oral	600	0.6
Mouse Intraperitoneal	360	0.58
Mouse Intravenous	150	0.64
Mouse Subcutaneous	110	0.43

ACDLabs models
Reliability index: <0.3 = Not reliable prediction quality; 0.3-0.5 = borderline prediction quality; 0.5-0.75 = moderate prediction quality; >0.75 = high prediction quality.

MRDD in Humans

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
MRDD in Humans ≤ 2.69 mg/kg-bw/d		NEG_OUT	INC_OUT	NEG_OUT	NEG_IN

DTU-developed models
Model based on data on pharmaceuticals. Maximum recommended daily dose in pharmaceutical clinical trials employing primarily oral route of exposure and daily treatments, usually for 3-12 months.

Irritation and Sensitization

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Severe Skin Irritation in Rabbit		NEG_OUT	INC_OUT	POS_OUT	NEG_IN
Skin sensitisation GHS/CLP at least Cat. 1, LLNA-based (open data only)				INC_OUT	
Skin sensitisation GHS/CLP at least Cat. 1, LLNA-based (open data and REACH-registrations)	N/A			INC_OUT	
Skin sensitisation GHS/CLP at least Cat. 1, LLNA-based, only negative predictions (open data only)				N/A	
Skin sensitisation GHS/CLP Cat. 1A, LLNA-based (open data only)				INC_OUT	
Skin sensitisation GHS/CLP Cat. 1A, LLNA-based (open data and REACH-registrations)	N/A			INC_OUT	
Skin sensitisation GHS/CLP Cat. 1A, LLNA-based, only positive predictions (open data and REACH-registrations)	N/A			N/A	
Allergic Contact Dermatitis in Guinea Pig and Human*	N/A	INC_OUT	INC_OUT	INC_OUT	POS_OUT
Respiratory Sensitisation in Humans		INC_OUT	POS_OUT	POS_OUT	NEG_OUT

DTU-developed models
**Based on commercial training set*

Protein binding by OASIS, alerts in:	
- parent only	No alert found
- metabolites from skin metabolism simulator only	
- metabolites from auto-oxidation simulator only	
Protein binding by OECD, alerts in:	
- parent only	No alert found
- metabolites from skin metabolism simulator only	
- metabolites from auto-oxidation simulator only	
Protein binding potency Cys (DRPA 13%), alerts in:	
- parent only	DPRA less than 9% (DPRA 13%) >> No protein binding alert
- metabolites from skin metabolism simulator only	
- metabolites from auto-oxidation simulator only	
Protein binding potency Lys (DRPA 13%), alerts in:	
- parent only	DPRA less than 9% (DPRA 13%) >> No protein binding alert
- metabolites from skin metabolism simulator only	
- metabolites from auto-oxidation simulator only	
Keratinocyte gene expression, alerts in:	
- parent only	Not possible to classify according to these rules
- metabolites from skin metabolism simulator only	
- metabolites from auto-oxidation simulator only	
Protein binding potency GSH, alerts in:	
- parent only	Not possible to classify according to these rules (GSH)

OECD QSAR Toolbox v.4.1 profilers
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

Endocrine and Molecular Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Estrogen Receptor α Binding, Full training set (Human *in vitro*)		INC_OUT	INC_OUT	NEG_OUT	NEG_OUT
Estrogen Receptor α Binding, Balanced Training Set (Human *in vitro*)		INC_OUT	INC_OUT	NEG_OUT	NEG_OUT
Estrogen Receptor α Activation (Human *in vitro*)		INC_OUT	INC_OUT	NEG_OUT	NEG_OUT
Estrogen Receptor Activation, CERAPP data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Androgen Receptor Inhibition (Human *in vitro*)		NEG_OUT	NEG_OUT	NEG_OUT	NEG_IN
Androgen Receptor Binding, CoMPARA data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Androgen Receptor Inhibition, CoMPARA data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Androgen Receptor Activation, CoMPARA data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Thyroperoxidase (TPO) inhibition QSAR1 (Rat *in vitro*)		N/A	N/A	INC_OUT	N/A
Thyroperoxidase (TPO) inhibition QSAR2 (Rat *in vitro*)		N/A	N/A	INC_OUT	N/A
Sodium/iodide symporter (NIS), higher sensitivity		N/A	N/A	INC_OUT	N/A
Sodium/iodide symporter (NIS), higher specificity		N/A	N/A	INC_OUT	N/A
Thyroid Receptor α Binding (Human *in vitro*)					
mg/L			22574.56	1533.555	21.13583
μM			159955.8	10866.25	149.7614
Positive for IC_{50} ≤ 10 μM					
Positive for IC_{50} ≤ 100 μM					
Domain		OUT	OUT	OUT	OUT
Thyroid Receptor β Binding (Human *in vitro*)					
mg/L			4566.88	28.29107	99.36178
μM			32359.38	200.4611	704.0443
Positive for IC_{50} ≤ 10 μM					
Positive for IC_{50} ≤ 100 μM					
Domain		OUT	OUT	OUT	OUT
Arylhydrocarbon (AhR) Activation – Rational final model (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Arylhydrocarbon (AhR) Activation – Random final model (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Pregnane X Receptor (PXR) Binding (Human *in vitro*)	N/A	INC_OUT	INC_OUT	NEG_OUT	NEG_OUT
Pregnane X Receptor (PXR) Binding (Human *in vitro*) NEW		N/A	N/A	INC_OUT	N/A
Pregnane X Receptor (PXR) Activation (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Pregnane X Receptor (PXR) Activation (Rat *in vitro*)		N/A	N/A	INC_OUT	N/A
CYP3A4 Induction (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Constitutive Androstane Receptor (CAR) Activation at max. 20 μM (*in vitro*)		N/A	N/A	INC_OUT	N/A
Constitutive Androstane Receptor (CAR) Activation at max. 50 μM (*in vitro*)		N/A	N/A	INC_OUT	N/A
Constitutive Androstane Receptor (CAR) Inhibition at max. 20 μM (*in vitro*)		N/A	N/A	INC_OUT	N/A
Constitutive Androstane Receptor (CAR) Inhibition at max. 50 μM (*in vitro*)	NEG	N/A	N/A	INC_OUT	N/A

DTU-developed models

Estrogen Receptor Binding, alerts in:	
- parent only	Non binder, non cyclic structure
- metabolites from *in vivo* Rat metabolism simulator only	Non binder, non cyclic structure
- metabolites from Rat liver S9 metabolism simulator only	Non binder, non cyclic structure
rtER Expert System - USEPA, alerts in:	
- parent only	No alert found
- metabolites from *in vivo* Rat metabolism simulator only	No alert found
- metabolites from Rat liver S9 metabolism simulator only	No alert found

OECD QSAR Toolbox v.4.2 profilers
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

Developmental Toxicity

	Battery	CASE Ultra	Leadscope	SciQSAR
Teratogenic Potential in Humans	POS_OUT	INC_OUT	INC_OUT	POS_IN

DTU-developed models based on commercial training set

Genotoxicity - Structural Alerts for DNA Reactivity

	Battery	CASE Ultra	Leadscope	SciQSAR
Ashby Structural Alerts	POS_OUT	POS_OUT	POS_OUT	POS_IN

DTU-developed models based on commercial training set

DNA binding by OASIS, alerts in:	
- parent only	No alert found
DNA binding by OECD, alerts in:	
- parent only	No alert found

OECD QSAR Toolbox v.4.2 profilers
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

In vitro Genotoxicity - Bacterial Reverse Mutation Test (Ames test)

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Ames test in S. typhimurium (*in vitro*)		NEG_OUT	NEG_OUT	NEG_OUT	NEG_IN
*Direct Acting Mutagens (without S9)	N/A	POS_OUT	INC_OUT	INC_OUT	POS_IN
*Base-Pair Ames Mutagens	N/A	NEG_OUT	INC_OUT	POS_OUT	NEG_IN
*Frameshift Ames Mutagens	N/A	NEG_OUT	INC_OUT	NEG_OUT	NEG_IN
*Potent Ames Mutagens, Reversions ≥ 10 Times Controls	N/A	POS_OUT	POS_OUT	NEG_OUT	POS_IN

DTU-developed models
* The four models (Direct Acting mutagens (without S9), Base-Pair Ames Mutagens, Frameshift Ames Mutagens, Potent Ames Mutagens) should not be used to determine if substances are Ames mutagens, but can be used for indication of mechanism or potency for cases where the main Ames model (Ames test in S. typhimurium (*in vitro*)) is POS_IN.

	VEGA	Mut. / Non-mut. scores	Used models
Mutagenicity consensus	NEG	0.05 / 0.15	4

Mutagenicity (Ames) consensus model version 1.0.2 contained in VEGA version 1.1.4 with calculation core version 1.2.4
Prediction: POS = Mutagenic, NEG = Non-mutagenic.

VEGA

ISS	CAESAR	SarPy	KNN
NEG_Low	POS_Low	POSS.NEG_Low	NEG_Low

Four individual models in mutagenicity consensus model version 1.0.2 contained in VEGA version 1.1.4 with calculation core version 1.2.4
Prediction: POS = Mutagenic, NEG = Non-mutagenic, SUSP.POS = Suspected mutagenic, POSS.NEG = Possible Non-mutagenic, Exp = experimental value, Good = Good reliability, Mod = Moderate reliability, Low = Low reliability.

DNA alerts for AMES by OASIS, alerts in:	
- parent only	No alert found
In vitro mutagenicity (Ames test) alerts by ISS, alerts in:	
- parent only	No alert found

OECD QSAR Toolbox v.4.2 profilers
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

Other *in vitro* Genotoxicity Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Chromosome Aberrations in Chinese Hamster Ovary (CHO) Cells*	N/A	NEG_OUT	INC_OUT	INC_OUT	NEG_IN
Chromosome Aberrations in Chinese Hamster Lung (CHL) Cells		POS_OUT	POS_OUT	INC_OUT	POS_IN
Mutations in Thymidine Kinase Locus in Mouse Lymphoma Cells		INC_OUT	POS_OUT	POS_OUT	NEG_OUT
Mutations in HGPRT Locus in Chinese Hamster Ovary (CHO) Cells		INC_OUT	POS_OUT	NEG_OUT	POS_OUT
Unscheduled DNA Synthesis (UDS) in Rat Hepatocytes		INC_OUT	INC_OUT	NEG_OUT	INC_OUT
Syrian Hamster Embryo (SHE) Cell Transformation		POS_OUT	INC_OUT	INC_OUT	POS_IN

DTU-developed models
**Based on commercial training set*
HGPRT: Hypoxanthine-guanine phosphoribosyltransferase

DNA alerts for CA and MNT by OASIS, alerts in:	
- parent only	No alert found
Protein binding alerts for Chromosomal aberration by OASIS, alerts in:	
- parent only	No alert found

OECD QSAR Toolbox v.4.2 profilers
CA: Chromosomal aberration, MNT: Micronucleus test
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

In vivo Genotoxicity Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Sex-Linked Recessive Lethal (SLRL) Test in Drosophila m.		NEG_OUT	INC_OUT	INC_OUT	NEG_IN
Micronucleus Test in Mouse Erythrocytes		NEG_OUT	INC_OUT	NEG_OUT	NEG_IN
Dominant Lethal Mutations in Rodents		NEG_OUT	INC_OUT	NEG_OUT	NEG_IN
Sister Chromatid Exchange in Mouse Bone Marrow Cells		INC_OUT	INC_OUT	POS_OUT	INC_OUT
Comet Assay in Mouse		POS_OUT	POS_OUT	POS_OUT	POS_IN

DTU-developed models

In vivo mutagenicity (Micronucleus) alerts by ISS, alerts in:	
- parent only	No alert found

OECD QSAR Toolbox v.4.2 profilers
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

Carcinogenicity

	E Ultra	Leadscope
FDA RCA Cancer Male Rat	NEG_OUT	INC_OUT
FDA RCA Cancer Female Rat	NEG_OUT	INC_OUT
FDA RCA Cancer Rat	NEG_OUT	INC_OUT
FDA RCA Cancer Male Mouse	NEG_OUT	INC_OUT
FDA RCA Cancer Female Mouse	NEG_OUT	INC_OUT
FDA RCA Cancer Mouse	NEG_OUT	INC_OUT
FDA RCA Cancer Rodent	NEG_OUT	INC_OUT

Commercial models from CASE Ultra and Leadscope
FDA RCA: Data from US Food and Drug Administration as part of Research Cooperation Agreement

Carcinogenicity (genotox and nongenotox) alerts by ISS, alerts in:	
- parent only	No alert found
Oncologic Primary Classification, alerts in:	
- parent only	Organophosphorus Type Compounds

OECD QSAR Toolbox v.4.2 profilers
Profiler predictions are supporting information to be used together with the relevant QSAR predictions

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Liver Specific Cancer in Rat or Mouse		INC_OUT	INC_OUT	NEG_OUT	INC_OUT

DTU-developed models

Abbreviations

INC: inconclusive. A definite call within the defined applicability domain could not be made.

NEG: negative

POS: positive

IN: inside applicability domain

OUT: outside applicability domain

Exp: Experimental values, from EpiSuite experimental databases or DK DTU QSAR models training sets.

N/A: Not applicable, either because training set data cannot be released for commercial or proprietary models / training sets, or because the model was not developed in a given QSAR software (i.e. a given prediction is not available as the model version does not exist).

Important notes

This is an automatically generated report from the Danish (Q)SAR Database, http://qsar.food.dtu.dk.

For predictions from CASE Ultra, Leadscope, SciQSAR as well as the Acute toxicity in rodent from ACDLabs information on the software versions can be found in the QMRFs. For the other predicted properties the software versions are:

EPI MPBPWIN v1.43

EPI HENRYWIN v3.20

EPI WSKOW v1.42

EPI WATERNT v1.01

EPI KOAWIN v1.10

EPI AEROWIN v1.00

EPI KOCWIN v2.00

EPI Level III Fugacity Model (EPI Suite v4.11)

EPI STPWIN (EPI Suite v4.11)

EPI AOPWIN v1.92

EPI BIOWIN v4.10

EPI BCFBAF v3.01

EPI ECOSAR v1.11

EPI DERMWIN v2.02

ACD/ ToxSuite 2.95.1 Ionization\pKa

ACD/ ToxSuite 2.95.1 Ionization\ LogD

ACD/ ToxSuite 2.95.1

It is recommended to run the latest version of the EPI Suite Programs in preference of the predictions given in this document when these endpoints are of importance and new versions have been released from the United States Environmental Protection Agency in comparisons. EPI Suite can be downloaded from the US EPA homepage: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

For further information on the applied systems, see the following homepages:

Case Ultra: http://www.multicase.com/case-ultra

Leadscope: http://www.leadscope.com/

SciQSAR: http://lhasa-llc.com/

ToxSuite: http://www.acdlabs.com/

Bilag B: Data fra CompTox Chemicals Dashboard

Physchem prop.

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Polarizability	-	12.9 (1)	-	12,9	-	12,9	Å^3
Henry's Law	-	1.70e-7 (1)	-	0,00000017	-	0,00000017	atm-m3/mole
ReadyBiodeg	-	0.00 (1)	-	0	-	0	Binary 0/1
Boiling Point	-	196 (3)	-	181	-	162 to 246	°C
Flash Point	-	51.9 (1)	-	51,9	-	51,9	°C
Melting Point	-	22.1 (2)	-	22,1	-	-63.8 to 108	°C
Molar Refractivity	-	32.5 (1)	-	32,5	-	32,5	cm^3
Molar Volume	-	110 (1)	-	110	-	110	cm^3
Atmos. Hydroxylation Rate	-	2.40e-10 (1)	-	2,4E-10	-	2,4E-10	cm3/molecule* sec
Biodeg. Half-Life	-	5.50 (1)	-	5,5	-	5,5	days
Fish Biotrans. Half-Life (Km)	-	0.117 (1)	-	0,117	-	0,117	days
Surface Tension	-	50.9 (1)	-	50,9	-	50,9	dyn/cm
Density	-	1.28 (1)	-	1,28	-	1,28	g/cm^3
Bioconcentration Factor	-	2.63 (1)	-	2,63	-	2,63	L/kg
Soil Adsorp. Coeff. (Koc)	-	3.02 (1)	-	3,02	-	3,02	L/kg
LogD5.5	-	0.150 (1)	-	0,15	-	0,15	Log10 unitless
LogD7.4	-	0.110 (1)	-	0,11	-	0,11	Log10 unitless
liquid chromatography Retention Time	-	0.00 (1)	-	0	-	0	min
Vapor Pressure	-	1.09 (2)	-	1,09	-	1.51e-4 to 2.19	mmHg
Water Solubility	-	0.579 (3)	-	0,399	-	0.186 to 1.15	mol/L
Index of Refraction	-	1.50 (1)	-	1,5	-	1,5	-
LogKoa: Octanol-Air	-	5.88 (1)	-	5,88	-	5,88	-
LogKow: Octanol-Water	-	-5.38e-2 (4)	-	0,175	-	-0.768 to 0.203	-
pKa Acidic Apparent	-	8.43 (1)	-	8,43	-	8,43	-

Env. Fate/Transport

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Atmos. Hydroxylation Rate	2.44e-10 (1)	2.40e-10 (1)	2,44E-10	2,4E-10	2.44e-10,2.44e-10	2.398832919019495e-10,2.398832919019495e-10	cm3/molecule*sec
Biodeg. Half-Life		5.50 (1)		5,5		5.495408738576246,5.495408738576246	days
Fish Biotrans. Half-Life (Km)		0.117 (1)		0,117		0.11748975549395294,0.11748975549395294	days
Bioconcentration Factor		2.63 (1)		2,63		2.6302679918953817,2.6302679918953817	L/kg
Soil Adsorp. Coeff. (Koc)		3.02 (1)		3,02		3.019951720402016,3.019951720402016	L/kg

Bilag C: Data fra NORMAN Ecotoxicology Database

Norman SusDat ID:	**NS00051691**
Name:	O,O-dimethyl thiophosphoramidate
CAS_RN:	CAS_RN: 17321-47-0
Validation Level:	Level 2
SMILES:	S=P(OC)(OC)N
SMILES Dashboard:	COP(N)(=S)OC
StdInChI:	InChI=1/C2H8NO2PS/c1-4-6(3,7)5-2/h1-2H3,(H2,3,7)
StdInChIKey:	NKYPKIVMIGIWOB-UHFFFAOYSA-N
MS_Ready_SMILES:	S=P(OC)(OC)N
MS_Ready_StdInChI:	InChI=1S/C2H8NO2PS/c1-4-6(3,7)5-2/h1-2H3,(H2,3,7)
MS_Ready_StdInChIKey:	NKYPKIVMIGIWOB-UHFFFAOYSA-N
Source:	
PubChem_CID:	87048
ChemSpiderID:	Not Retrieved
DTXSID:	DTXSID4027789
Molecular_Formula:	C2H8NO2PS
Monoiso_Mass:	141.001336126
[M+H]+:	142.0086
[M-H]-:	139.9941
Pred_RTI_Positive_ESI:	347.16
Uncertainty_RTI_pos:	Covered by Model
Pred_RTI_Negative_ESI:	93.29
Uncertainty_RTI_neg:	Covered by Model
Tetrahymena_pyriformis_toxicity:	2.18421509065004
IGC50_48_hr_ug/L:	922588.713570353
Uncertainty_Tetrahymena_pyriformis_toxicity:	Covered by Model
Daphnia_toxicity:	4.68654149436667
LC50_48_hr_ug/L:	2901.8952637697
Uncertainty_Daphnia_toxicity:	Covered by Model
Algae_toxicity:	3.42878069512003
EC50_72_hr_ug/L:	52534.2495700164
Uncertainty_Algae_toxicity:	Covered by Model
Pimephales_promelas_toxicity:	3.40343933207943
LC50_96_hr_ug/L:	55690.8563421935
Uncertainty_Pimephales_promelas_toxicity:	Covered by Model
logKow_EPISuite:	0.2
Exp_logKow_EPISuite:	NA
ChemSpider ID based on InChIKey_19032018:	Not Retrieved
alogp_ChemSpider:	Not Retrieved
xlogp_ChemSpider:	Not Retrieved
Lowest P-PNEC (QSAR) [ug/L]:	2.9
Species:	Daphnia magna
Uncertainty:	Covered by Model
ExposureScore_Water_KEMI:	0.29
ValidationLevel_KEMI:	2

Parameter	Original database entry	Final database entry
Test substance		
SUSDAT ID	00051691	00051691
CAS Number	CAS_RN: 17321-47-0	CAS_RN: 17321-47-0
Substance Name	O,O-dimethyl thiophosphoramidate	O,O-dimethyl thiophosphoramidate
Test item		
Purity [%]		
Quality target		
Institution / Authority who derived the PNEC	NORMAN	NORMAN
Country or Region the PNEC was derived for	Worldwide	Worldwide
PNEC type	P-PNEC pred	P-PNEC pred
PNEC type (country specific name)		
Regulatory context		
Compartment	freshwater	freshwater
Protection objective	freshwater aquatic life	freshwater aquatic life
Concentration specification		
Monitoring Frequency	annual average	annual average
Mixture RA Group	n.a.	n.a.
Underlying biotest		
Species name	Tetrahymena pyriformis	Tetrahymena pyriformis
Key endpoint	IC50	IC50
Effect measurement	growth rate	growth rate
Duration	48 h	48 h
Exposure Regime		
Effect concentration qualifier		
Effect concentration		
Measured or nominal concentrations		
Biotest ID	n.r.	n.r.
Quality evaluation		
Reliabilty of the key study	1	1
Reliability score system used	CRED	CRED
Reliabilty of the key study	NORMAN	NORMAN
PNEC derivation		
Derivation method	Deterministic	Deterministic
Applied AF	1000	1000
Justification	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)
PNEC Value	922.588713570353	922.588713570353
Remarks	n.a.	n.a.
Vote		
Expert	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.
PNEC Quality Class		
Date		
References and Sources		
Title of Dossier	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models
Bibliographic source	Environ. Sci.: Processes Impacts, 2017,19, 438-448	Environ. Sci.: Processes Impacts, 2017,19, 438-448
Link to Dossier	No	No
Link to Directive		
Data source name	NORMAN Suspect List Exchange	NORMAN Suspect List Exchange
Data source ID	n.a.	n.a.
Data source link	https://www.norman-network.com/nds/susdat/	https://www.norman-network.com/nds/susdat/
NORMAN PNEC ID	PNEC-ID-0198087	PNEC-ID-0198087
NORMAN Dataset ID	PNEC-DS-1	PNEC-DS-1
Publication Year	2017	2017

Parameter	Original database entry	Final database entry
Test substance		
SUSDAT ID	00051691	00051691
CAS Number	CAS_RN: 17321-47-0	CAS_RN: 17321-47-0
Substance Name	O,O-dimethyl thiophosphoramidate	O,O-dimethyl thiophosphoramidate
Test item		
Purity [%]		
Quality target		
Institution / Authority who derived the PNEC	NORMAN	NORMAN
Country or Region the PNEC was derived for	Worldwide	Worldwide
PNEC type	P-PNEC pred	P-PNEC pred
PNEC type (country specific name)		
Regulatory context		
Compartment	freshwater	freshwater
Protection objective	freshwater aquatic life	freshwater aquatic life
Concentration specification		
Monitoring Frequency	annual average	annual average
Mixture RA Group	Crustacean	crustacean
Underlying biotest		
Species name	Daphnia magna	Daphnia magna
Key endpoint	LC50	LC50
Effect measurement	Mortality	Mortality
Duration	48 h	48 h
Exposure Regime		
Effect concentration qualifier		
Effect concentration		
Measured or nominal concentrations		
Biotest ID	n.r.	n.r.
Quality evaluation		
Reliabilty of the key study	1	1
Reliability score system used	CRED	CRED
Reliabilty of the key study	NORMAN	NORMAN
PNEC derivation		
Derivation method	Deterministic	Deterministic
Applied AF	1000	1000
Justification	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)
PNEC Value	2.9018952637697	2.9018952637697
Remarks	n.a.	n.a.
Vote		
Expert	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.
PNEC Quality Class		
Date		
References and Sources		
Title of Dossier	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models
Bibliographic source	Environ. Sci.: Processes Impacts, 2017,19, 438-448	Environ. Sci.: Processes Impacts, 2017,19, 438-448
Link to Dossier	No	No
Link to Directive		
Data source name	NORMAN Suspect List Exchange	NORMAN Suspect List Exchange
Data source ID	n.a.	n.a.
Data source link	https://www.norman-network.com/nds/susdat/	https://www.norman-network.com/nds/susdat/
NORMAN PNEC ID	PNEC-ID-0198088	PNEC-ID-0198088
NORMAN Dataset ID	PNEC-DS-1	PNEC-DS-1
Publication Year	2017	2017

Parameter	Original database entry	Final database entry
Test substance		
SUSDAT ID	00051691	00051691
CAS Number	CAS_RN: 17321-47-0	CAS_RN: 17321-47-0
Substance Name	O,O-dimethyl thiophosphoramidate	O,O-dimethyl thiophosphoramidate
Test item		
Purity [%]		
Quality target		
Institution / Authority who derived the PNEC	NORMAN	NORMAN
Country or Region the PNEC was derived for	Worldwide	Worldwide
PNEC type	P-PNEC pred	P-PNEC pred
PNEC type (country specific name)		
Regulatory context		
Compartment	freshwater	freshwater
Protection objective	freshwater aquatic life	freshwater aquatic life
Concentration specification		
Monitoring Frequency	annual average	annual average
Mixture RA Group	algae and plants	algae and plants
Underlying biotest		
Species name	Selenastrum capricornutum	Selenastrum capricornutum
Key endpoint	EC50	EC50
Effect measurement	immobilisation	immobilisation
Duration	72 h	72 h
Exposure Regime		
Effect concentration qualifier		
Effect concentration		
Measured or nominal concentrations		
Biotest ID	n.r.	n.r.
Quality evaluation		
Reliabilty of the key study	1	1
Reliability score system used	CRED	CRED
Reliabilty of the key study	NORMAN	NORMAN
PNEC derivation		
Derivation method	Deterministic	Deterministic
Applied AF	1000	1000
Justification	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)
PNEC Value	52.5342495700164	52.5342495700164
Remarks	n.a.	n.a.
Vote		
Expert	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.
PNEC Quality Class		
Date		
References and Sources		
Title of Dossier	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models
Bibliographic source	Environ. Sci.: Processes Impacts, 2017,19, 438-448	Environ. Sci.: Processes Impacts, 2017,19, 438-448
Link to Dossier	No	No
Link to Directive		
Data source name	NORMAN Suspect List Exchange	NORMAN Suspect List Exchange
Data source ID	n.a.	n.a.
Data source link	https://www.norman-network.com/nds/susdat/	https://www.norman-network.com/nds/susdat/
NORMAN PNEC ID	PNEC-ID-0198089	PNEC-ID-0198089
NORMAN Dataset ID	PNEC-DS-1	PNEC-DS-1
Publication Year	2017	2017

Parameter	Original database entry	Final database entry
Test substance		
SUSDAT ID	00051691	00051691
CAS Number	CAS_RN: 17321-47-0	CAS_RN: 17321-47-0
Substance Name	O,O-dimethyl thiophosphoramidate	O,O-dimethyl thiophosphoramidate
Test item		
Purity [%]		
Quality target		
Institution / Authority who derived the PNEC	NORMAN	NORMAN
Country or Region the PNEC was derived for	Worldwide	Worldwide
PNEC type	P-PNEC pred	P-PNEC pred
PNEC type (country specific name)		
Regulatory context		
Compartment	freshwater	freshwater
Protection objective	freshwater aquatic life	freshwater aquatic life
Concentration specification		
Monitoring Frequency	annual average	annual average
Mixture RA Group	fish	fish
Underlying biotest		
Species name	Pimephales promelas	Pimephales promelas
Key endpoint	LC50	LC50
Effect measurement	mortality	mortality
Duration	96 h	96 h
Exposure Regime		
Effect concentration qualifier		
Effect concentration		
Measured or nominal concentrations		
Biotest ID	n.r.	n.r.
Quality evaluation		
Reliabilty of the key study	1	1
Reliability score system used	CRED	CRED
Reliabilty of the key study	NORMAN	NORMAN
PNEC derivation		
Derivation method	Deterministic	Deterministic
Applied AF	1000	1000
Justification	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)	One predicted short-term L(E)C50 from each of three trophic levels (i.e. base set)
PNEC Value	55.6908563421935	55.6908563421935
Remarks	n.a.	n.a.
Vote		
Expert	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.	Aalizadeh, R. von der Ohe, P. and Thomaidis, N.S.
PNEC Quality Class		
Date		
References and Sources		
Title of Dossier	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models	Contaminants on the Water Flea Daphnia magna by Ant Colony Optimization - Support Vector Machine QSTR models
Bibliographic source	Environ. Sci.: Processes Impacts, 2017,19, 438-448	Environ. Sci.: Processes Impacts, 2017,19, 438-448
Link to Dossier	No	No
Link to Directive		
Data source name	NORMAN Suspect List Exchange	NORMAN Suspect List Exchange
Data source ID	n.a.	n.a.
Data source link	https://www.norman-network.com/nds/susdat/	https://www.norman-network.com/nds/susdat/
NORMAN PNEC ID	PNEC-ID-0198090	PNEC-ID-0198090
NORMAN Dataset ID	PNEC-DS-1	PNEC-DS-1
Publication Year	2017	2017