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The new ECHA CHEM database has been released by ECHA, and it now contains all REACH registration data. There are more details on the transition of ECHA's published data to ECHA CHEM <u>here</u>.

Access ECHA CHEM

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	REACH	
Fuels, diesel		
EC number: 269-8227   CAS number: 68334-30-5 A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numb range of C9 through C20 and boiling in the range of approximately 163°C to 357°C (325°F to 675°F).	oers predominar	ntly in the



Environmental fate & pathways Bioaccumulation: aquatic / sediment

### Administrative data

Endpoint:	bioaccumulation: aquatic / sediment
Type of information:	(Q)SAR
Adequacy of study:	weight of evidence
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	other: Regulatory accepted QSAR method for organic chemicals properties assessment.
Justification for type of information:	QSAR prediction: migrated from IUCLID 5.6

#### Data source

Reference	
Reference Type:	other company data
Title:	Unnamed
Year:	2010

## Materials and methods

Test guideline	
Qualifier:	according to guideline
Guideline:	other: QSAR method
Principles of method if other than guideline:	QSAR method
GLP compliance:	no
Remarks:	not applicable to QSAR models

**Test material** 

Test material information			
Constituent 1			
	Reference substance name:	data for components	
	IUPAC Name:	data for components	
Details on test ma	aterial: data for cor	nponents	

# **Results and discussion**

## Any other information on results incl. tables

Overview of QSAR data on aquatic bioaccumulation of Diesel Fuelcomponents

Method	Results	Remarks	Reference
Hovano C	<sub>6</sub> H <sub>14</sub> (CAS No. 110-54-3)		
lexalle, o	6114(CAS NO. 110 34 3)		
QSAR estimate	Estimated Log BCF =2.24; BCF =174 L/kg wet-wt	2 (reliable with	USEPA (EPI
BCFBAF v.3.00	L/Kg wet-wi	restrictions)	Suite v.4.00)
		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.23 Bioaccumulation factor=169.81	Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	Software Tool),
Heptane, (	C <sub>7</sub> H <sub>16</sub> (CAS No. 142-82-5)		
QSAR	Estimated Log BCF =2.74; BCF =552	2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	L/kg wet-wt	restrictions)	Suite v.4.00)
		key study	
Due die te d	Discourse detion forten la r10	(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.57 Bioaccumulation factor=367.93	Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	Software Tool),
Octane, Ca	BH <sub>18</sub> (CAS No. 111-65-9)		
QSAR	Estimated Log BCF =3.08; BCF	2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	=1220 L/kg wet-wt	restrictions)	Suite v.4.00)
		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.91 Bioaccumulation factor=809.39	Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
Nonane, C	<sub>9</sub> H <sub>20</sub> (CAS No. 111-84-2)		

estimate	Estimated Log BCF =2.02; BCF =10 L/kg wet-wt	15 2 (reliable with	USEPA (EPI
BCFBAF	L/ kg wet-wi	restrictions)	Suite v.4.00)
v.3.00			
		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.81	Peer reviewed data referred in the US EPA	US EPA, T.E.S.T. (Toxicity
	Bioaccumulation factor=653.02		estimation Software Tool),
Decane, C	C <sub>10</sub> H <sub>22</sub> (CAS No. 124-18-5)		
QSAR	Estimated Log BCF =1.60; BCF	2 (reliable with	USEPA (EPI
estimate	=39.7 L/kg wet-wt	restrictions)	Suite v.4.00)
BCFBAF v.3.00		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.87	Peer reviewed data referred in the US EPA	US EPA, T.E.S.T. (Toxicity
	2.87 Bioaccumulation factor=748.28		(Toxicity estimation Software Tool), 2010
Hendecan	ne, C <sub>11</sub> H <sub>24</sub> (CAS No. 1120-21-4)	)	
QSAR	Estimated Log BCF =2.08; BCF	2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	=121 L/kg wet-wt	restrictions)	Suite v.4.00)
		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.83 Bioaccumulation factor=683.30	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
	2.83	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model	(Toxicity estimation Software Tool),
Predicted	2.83	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical	(Toxicity estimation Software Tool),
Predicted	2.83 Bioaccumulation factor=683.30 e, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3)	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	(Toxicity estimation Software Tool), 2010
Predicted Dodecane QSAR estimate BCFBAF	2.83 Bioaccumulation factor=683.30	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical	(Toxicity estimation Software Tool),
Predicted Dodecane QSAR estimate BCFBAF	2.83 Bioaccumulation factor=683.30 e, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances 2 (reliable with	(Toxicity estimation Software Tool), 2010 USEPA (EPI
Predicted Dodecane QSAR estimate BCFBAF	2.83 Bioaccumulation factor=683.30 e, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances 2 (reliable with restrictions)	(Toxicity estimation Software Tool), 2010 USEPA (EPI
Predicted Dodecane QSAR estimate BCFBAF v.3.00	2.83 Bioaccumulation factor=683.30 c, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF =208 L/kg wet-wt Bioaccumulation factor Log10 =	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data	(Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T.
Predicted Dodecane QSAR estimate BCFBAF v.3.00	2.83 Bioaccumulation factor=683.30 C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF =208 L/kg wet-wt	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA	(Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),
Predicted Dodecane QSAR estimate BCFBAF v.3.00 Predicted	2.83 Bioaccumulation factor=683.30 c, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF =208 L/kg wet-wt Bioaccumulation factor Log10 = 2.60	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical	(Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),
Predicted Dodecane OSAR estimate BCFBAF v.3.00 Predicted	2.83 Bioaccumulation factor=683.30 c, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF =208 L/kg wet-wt Bioaccumulation factor Log10 = 2.60 Bioaccumulation factor=395.92 c, C <sub>13</sub> H <sub>28</sub> (CAS No. 629-50-5)	<ul> <li>(Q)SAR</li> <li>Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances</li> <li>2 (reliable with restrictions)</li> <li>key study</li> <li>(Q)SAR</li> <li>Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances</li> </ul>	(Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
Predicted Dodecane QSAR estimate BCFBAF v.3.00 Predicted Tridecane QSAR estimate	2.83 Bioaccumulation factor=683.30 c, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF =208 L/kg wet-wt Bioaccumulation factor Log10 = 2.60 Bioaccumulation factor=395.92	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical	(Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),
Predicted Dodecane QSAR estimate BCFBAF v.3.00 Predicted Tridecane	2.83 Bioaccumulation factor=683.30 c, C <sub>12</sub> H <sub>26</sub> (CAS No. 112-40-3) Estimated Log BCF =2.32; BCF =208 L/kg wet-wt Bioaccumulation factor Log10 = 2.60 Bioaccumulation factor=395.92 c, C <sub>13</sub> H <sub>28</sub> (CAS No. 629-50-5) Estimated Log BCF =2.73; BCF	<ul> <li>(Q)SAR</li> <li>Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances</li> <li>2 (reliable with restrictions)</li> <li>key study</li> <li>(Q)SAR</li> <li>Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances</li> <li>2 (reliable with</li> </ul>	(Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010

	Bioaccumulation factor Log10 = 2.56 Bioaccumulation factor=363.73	Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
Tetradeca	ane, C <sub>14</sub> H <sub>30</sub> (CAS No. 629-59-4)		
QSAR	Estimated Log BCF =3.43; BCF =	2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	2690 L/kg wet-wt	restrictions) key study	Suite v.4.00)
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 =	Peer reviewed data	US EPA, T.E.S.T.
	2.51 Bioaccumulation factor=322.52	referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	(Toxicity estimation Software Tool), 2010
Pentadec	ane, C <sub>15</sub> H <sub>32</sub> (CAS No. 629-62-9	)	
QSAR	Estimated Log BCF =3.18; BCF =	2 (reliable with	USEPA (EPI
estimate	1520 L/kg wet-wt	restrictions)	Suite v.4.00)
BCFBAF v.3.00		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.59	Peer reviewed data referred in the US EPA	US EPA, T.E.S.T. (Toxicity estimation
	Bioaccumulation factor=386.34	Common and a second	Software Teel)
		for regulatory assessment of chemical substances	Software Tool), 2010
Hexadeca	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3)	assessment of chemical substances	
Hexadeca	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3) Estimated Log BCF =2.940; BCF =	assessment of chemical substances	
	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3)	assessment of chemical substances	2010
QSAR estimate BCFBAF	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3) Estimated Log BCF =2.940; BCF =	assessment of chemical substances 2 (reliable with	2010 USEPA (EPI
QSAR estimate BCFBAF v.3.00	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3) Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
QSAR estimate BCFBAF	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3) Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 =	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),
QSAR estimate BCFBAF v.3.00 Predicted	ane, C <sub>16</sub> H <sub>34</sub> (CAS No. 544-76-3) Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),
QSAR estimate BCFBAF v.3.00 Predicted Heptadec QSAR	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82 cane, $C_{17}H_{36}$ (CAS No. 629-78-7 Estimated Log BCF =2.699; BCF =	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),
QSAR estimate BCFBAF v.3.00 Predicted Heptadec	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
QSAR estimate BCFBAF v.3.00 Predicted Heptadec QSAR estimate BCFBAF	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82 cane, $C_{17}H_{36}$ (CAS No. 629-78-7 Estimated Log BCF =2.699; BCF =	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances ) 2 (reliable with	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010 USEPA (EPI
QSAR estimate BCFBAF v.3.00 Predicted Heptadec QSAR estimate BCFBAF	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82 cane, $C_{17}H_{36}$ (CAS No. 629-78-7 Estimated Log BCF =2.699; BCF =	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances ) 2 (reliable with restrictions)	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010 USEPA (EPI
QSAR estimate BCFBAF v.3.00 Predicted Heptadec QSAR estimate BCFBAF	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82 cane, $C_{17}H_{36}$ (CAS No. 629-78-7 Estimated Log BCF =2.699; BCF =	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances ) 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation
QSAR estimate BCFBAF v.3.00 Predicted Heptadec QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82 ane, C <sub>17</sub> H <sub>36</sub> (CAS No. 629-78-7 Estimated Log BCF =2.699; BCF = 500.4 L/kg wet-wt Bioaccumulation factor Log10 = 2.48	assessment of chemical substances 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances ) 2 (reliable with restrictions) key study (Q)SAR Peer reviewed data referred in the US EPA	2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010 USEPA (EPI Suite v.4.00) US EPA, T.E.S.T. (Toxicity estimation Software Tool),

QSAR	Estimated Log BCF =2.459; BCF =	2 (reliable with	USEPA (EPI
estimate	287.5 L/kg wet-wt	restrictions)	Suite v.4.00)
BCFBAF v.3.00			
		key study	
		(Q)SAR	
Predicted	Discoursulation factor-205.60	1 I I I I I I I I I I I I I I I I I I I	US EPA, T.E.S.T. (Toxicity estimation
		for regulatory assessment of chemical substances	Software Tool), 2010
Nonadeca	ane, C <sub>19</sub> H <sub>40</sub> (CAS No. 629-92-5)		
QSAR		2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	165.2 L/kg wet-wt	restrictions)	Suite v.4.00)
v.3.00		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 =	Peer reviewed data referred in the US EPA	US EPA, T.E.S.T.
	2.65 Bioaccumulation factor=444.50		(Toxicity estimation Software Tool), 2010
Eicosane,	C <sub>20</sub> H <sub>42</sub> (CAS No. 112-95-8)		
QSAR	Log BCF =1.98; BCF = 94.9 L/kg wet	2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	wt	restrictions)	Suite v.4.00)
		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=462.79		US EPA, T.E.S.T. (Toxicity estimation
		for regulatory assessment of chemical substances	Software Tool), 2010
Toluene, C	C <sub>7</sub> H <sub>8</sub> (CAS No. 108-88-3)		
QSAR	Estimated Log BCF =1.47; BCF	2 (reliable with	USEPA (EPI
estimate BCFBAF v.3.00	=29.4 L/kg wet-wt	restrictions)	Suite v.4.00)
v.3.00		key study	
		(Q)SAR	
Predicted	Bioaccumulation factor Log10 = 1.75	Peer reviewed data referred in the US EPA	US EPA, T.E.S.T. (Toxicity
	Bioaccumulation factor=56.68		estimation Software Tool),
Ethylbenz	ene, C <sub>8</sub> H <sub>10</sub> (CAS No. 100-41-4)		
QSAR	Estimated Log BCF=1.75; BCF =55.6	2 (reliable with	USEPA (EPI
estimate	L/kg wet-wt	restrictions)	Suite v.4.00)
BCFBAF			
BCFBAF v.3.00		key study	

Predicted	Bioaccumulation factor Log10 = 2.11 Bioaccumulation factor=128.50	Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
p-Xylene,	C <sub>8</sub> H <sub>10</sub> (CAS No. 106-42-3)		
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =1.75; BCF =55.6 L/kg wet-wt	2 (reliable with restrictions)	USEPA (EPI Suite v.4.00)
		key study (Q)SAR	
Predicted	Bioaccumulation factor Log10 = 2.08 Bioaccumulation factor=121.60	Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical substances	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
o-Xylene,	C <sub>8</sub> H <sub>10</sub> (CAS No. 95-47-6)		
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =1.73; BCF = 53.2 L/kg wet-wt	2 (reliable with restrictions) key study	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.08 Bioaccumulation factor=120.50	(Q)SAR Peer reviewed data referred in the US EPA developed QSAR model for regulatory assessment of chemical	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010

## Applicant's summary and conclusion

Conclusions:

Generally, a BCF in fish of  $\geq$  500 is indicative of the potential to bioconcentrate for classification purposes in accordance with CLP/GHS criteria. The BCF values estimated for Diesel Fuel suggest some bioaccumulation potential for some paraffin Diesel Fuel components.

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