REACH

Fuels, diesel

EC number: 269-822-7 | CAS number: 68334-30-5

A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C20 and boiling in the range of approximately 163°C to 357°C (325°F to 675°F).

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 material:	data for components

Results and discussion

Any other information on results incl. tables

Overview of QSAR data on aquatic bioaccumulation ofDiesel Fuelcomponents

Method	Results	Remarks	Reference
Hexane, C_6H_{14}(CAS No. 110-54-3)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.24; BCF =174 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
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	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
Heptane, C_7H_{16}(CAS No. 142-82-5)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.74; BCF =552 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
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	US EPA, T.E.S.T. (Toxicity estimation Software Tool), 2010
Octane, C_8H_{18}(CAS No. 111-65-9)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =3.08; BCF =1220 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
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_9H_{20}(CAS No. 111-84-2)			

QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.02; BCF =105 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.81 Bioaccumulation factor=653.02	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
Decane, $C_{10}H_{22}$(CAS No. 124-18-5)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =1.60; BCF =39.7 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.87 Bioaccumulation factor=748.28	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
Hendecane, $C_{11}H_{24}$(CAS No. 1120-21-4)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.08; BCF =121 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.83 Bioaccumulation factor=683.30	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
Dodecane, $C_{12}H_{26}$(CAS No. 112-40-3)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.32; BCF =208 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.60 Bioaccumulation factor=395.92	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
Tridecane, $C_{13}H_{28}$(CAS No. 629-50-5)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.73; BCF =537 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)

Predicted	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
Tetradecane, $C_{14}H_{30}$(CAS No. 629-59-4)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =3.43; BCF = 2690 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.51 Bioaccumulation factor=322.52	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
Pentadecane, $C_{15}H_{32}$(CAS No. 629-62-9)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =3.18; BCF = 1520 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.59 Bioaccumulation factor=386.34	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
Hexadecane, $C_{16}H_{34}$(CAS No. 544-76-3)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.940; BCF = 870.9 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=466.82	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
Heptadecane, $C_{17}H_{36}$(CAS No. 629-78-7)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.699; BCF = 500.4 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.48 Bioaccumulation factor=303.25	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
Octadecane, $C_{18}H_{38}$(CAS No. 593-45-3)			

QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.459; BCF = 287.5 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.59 Bioaccumulation factor=385.68	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
Nonadecane, $C_{19}H_{40}$(CAS No. 629-92-5)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =2.218; BCF = 165.2 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.65 Bioaccumulation factor=444.50	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
Eicosane, $C_{20}H_{42}$(CAS No. 112-95-8)			
QSAR estimate BCFBAF v.3.00	Log BCF =1.98; BCF = 94.9 L/kg wet wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.67 Bioaccumulation factor=462.79	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
Toluene, C_7H_8(CAS No. 108-88-3)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF =1.47; BCF =29.4 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 1.75 Bioaccumulation factor=56.68	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
Ethylbenzene, C_8H_{10}(CAS No. 100-41-4)			
QSAR estimate BCFBAF v.3.00	Estimated Log BCF=1.75; BCF =55.6 L/kg wet-wt	2 (reliable with restrictions) key study (Q)SAR	USEPA (EPI Suite v.4.00)

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_8H_{10}(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) key study (Q)SAR	USEPA (EPI Suite v.4.00)
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_8H_{10}(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 (Q)SAR	USEPA (EPI Suite v.4.00)
Predicted	Bioaccumulation factor Log10 = 2.08 Bioaccumulation factor=120.50	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

Applicant's summary and conclusion

Conclusions: Generally, a BCF in fish of ≥ 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.