REACH

Paraffin oils

EC number: 232-384-2 | CAS number: 8012-95-1
Liquid hydrocarbons from petroleum.

Toxicological information

Genetic toxicity: in vitro

001 Weight of evidence | (Q)SAR

Administrative data

Endpoint:	genetic toxicity in vitro
Remarks:	Type of genotoxicity: other: QSAR
Type of information:	(Q)SAR
Adequacy of study:	weight of evidence
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	other: Regulatory accepted model for assessment of chemical substances
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

Principles of method if other than guideline:	QSAR
GLP compliance:	no
Remarks:	not applicable to QSAR models
Type of assay:	other: QSAR

Test material

Test material information

Constituent 1

Reference substance name:	data for components
IUPAC Name:	data for components
Details on test material:	Mineral Paraffin Oil is a complex UVCB substance. Data for components.

Results and discussion

Any other information on results incl. tables

Overview of QSAR/SAR estimations on mutagenicity potential of Mineral Paraffin Oil

Method	Results	Remarks	Reference
Pentadecane, $C_{15}H_{32}$(CAS No. 629-62-9)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0

Predicted	Mutagenicity result: Mutagenicity Negative	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)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5

QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Henicosane, $C_{21}H_{44}$(CAS No. 629-94-7)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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

Docosane, $C_{22}H_{46}$(CAS No. 629-97-0)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Tricosane, $C_{23}H_{48}$(CAS No. 638-67-5)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Tetracosane, $C_{24}H_{50}$ (CAS No. 646-31-1)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0

QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Pentacosane, $C_{25}H_{52}$ (CAS No. 629-99-2)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Hexacosane, $C_{26}H_{54}$ (CAS No 630-01-3)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Heptacosane, $C_{27}H_{56}$ (CAS No. 593-49-7)			

CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Octacosane, $C_{28}H_{58}$ (CAS No. 630-02-4)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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
Nonacosane, $C_{29}H_{60}$ (CAS No. 630-03-5)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0

Predicted	Mutagenicity result: Mutagenicity Negative	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
Triacontane, $C_{30}H_{62}$(CAS No. 638-68-6)			
CAESAR QSAR model for Mutagenicity v.1.0.0.5	Activity: NON-Mutagen	Supportive data	CAESAR QSAR model for Mutagenicity v.1.0.0.5
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: Negative for genotoxic carcinogenicity. Negative for nongenotoxic carcinogenicity.	The decision logic is based on Benigni/Bossa rulebase (for mutagenicity and carcinogenicity)	Toxtree, v. 2.5.0
QSAR Method: Toxtree (Estimation of Toxic Hazard –A Decision Tree Approach) based on SMILES	Result: No alerts for micronucleus assay (Class II)	The decision logic is based on Structure Alerts fort he in vivo micronucleus assay in rodents	Toxtree, v. 2.5.0
Predicted	Mutagenicity result: Mutagenicity Negative	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: Screening of Mineral Paraffin Oil hydrocarbon components for mutagenicity/genotoxicity using several available QSAR models provide negative prediction results for this endpoint.