REACH

Fatty acids, C16 and C18-unsatd., triesters with trimethylolpropane

EC number: 270-287-7 | CAS number: 68424-27-1
This substance is identified by SDA Substance Name: C16 and C18 unsaturated trialkyl carboxylic acid trimethylolpropane triester and SDA Reporting Number: 09-015-00.

Toxicological information

Acute Toxicity: oral

001 Key | Other result type (JS Member) (Opt-out)

Administrative data

Endpoint:	acute toxicity: oral
Type of information:	other: data sharing dispute
Adequacy of study:	key study
Study period:	24 Jan - 12 Feb 2002
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	other: GLP-Guideline study with acceptable restrictions (no analytical purity data available)
Justification for type of information:	Guidance on registration Reference: ECHA-16-G-06-EN Publ.date:November 2016 Practical guide 2: How to report weight of evidence - Reference: ECHA-10-B-05-EN Publ.date: 24/03/2010 "Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals" (ECHA 2008) According to Article 13 of Regulation (EC) No. 1907/2006 "General Requirements for Generation of Information on Intrinsic Properties of substances", information on intrinsic properties of substances may be generated by means other than tests e.g. from information from structurally related substances (grouping or read-across), provided that conditions set out in Annex XI are met. Annex XI, "General rules for adaptation of this standard testing regime set out in Annexes VII to X" states that "substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity may be considered as a group, or 'category' of substances. This avoids the need to test every substance for every endpoint".Since the category concept is applied to the polyol esters, data gaps will be filled by interpolation, as part of a read across approach from a representative category member(s) to avoid unnecessary animal testing. Additionally, once the category concept is applied, substances will be classified and labelled on this basis.Therefore, based on the group concept, all available data on repeated dose toxicity do not meet the classification criteria according to Regulation. See Category Justification Document Point enclosed at 13.2

Cross-reference

Cross-reference 1

other: weight of evidence

Reason / purpose for cross-reference:	

Reference

Endpoint:	acute toxicity: oral
Type of information:	(Q)SAR
Adequacy of study:	weight of evidence
Study period:	November 2016
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	accepted calculation method
Justification for type of information:	Guidance on registration Reference: ECHA-16-G-06-EN Publ.date:November 2016 Practical guide 2: How to report weight of evidence - Reference: ECHA-10-B-05-EN Publ.date: 24/03/2010 "Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals" (ECHA 2008)
Reason / purpose for cross-reference:	other: weight of evidence
Reason / purpose for cross-reference:	other: weight of evidence
Reason / purpose for cross-reference:	other: weight of evidence
Qualifier:	according to guideline
Guideline:	other: REACH Guidance on Qsars and grouping of chemicals R.6 year 2008
Principles of method if other than guideline:	Consensus method: The predicted toxicity is estimated by taking an average of the predicted toxicities from the below QSAR methods (provided the predictions are within the respective applicability domains): Hierarchical method: The toxicity for a given query compound is estimated using the weighted average of the predictions from several different models. The different models are obtained by using Ward's method to divide the training set into a series of structurally similar clusters. A genetic algorithm based technique is used to generate models for each cluster. The models are generated prior to runtime. FDA method: The prediction for each test chemical is made using a new model that is fit to the chemicals that are most similar to the test compound. Each model is generated at runtime. Single model method: Predictions are made using a multilinear regression model that is fit to the training set (using molecular descriptors as independent variables) using a genetic algorithm based approach. The regression model is generated prior to runtime. Group contribution method: Predictions are made using a multilinear regression model that is fit to the training set (using molecular fragment counts as independent variables). The regression model is generated prior to runtime. Nearest neighbor method: The predicted toxicity is estimated by taking an average of the 3 chemicals in the training set that are most similar to the test chemical. User's Guide for T.E.S.T.(Toxicity Estimation Software Tool) T. Martin - U.S. EPA/National Risk Management Research Laboratory/Sustainable Technology Division, Cincinnati, OH 45268
Specific details on test material used for the study:	SMILES STRING C(CCCCCCC\C=C/CCCCCCCC)(=O)OCC(CC)(COC(CCCCCCC\C=C/CCCCCCCC)=O)COC(CCCCCCC\C=C/CCCCCCCC)=O
	Key result
Dose descriptor:	LD50
Effect level:	>= 28.981 other: mg/kg
Conclusions:	Oral rat LD50 mg/kg 28981,02

Cross-reference 2

Reason / purpose for cross-reference:	other: weight of evidence

Reference

Endpoint:	acute toxicity: oral
Type of information:	(Q)SAR
Adequacy of study:	weight of evidence
Study period:	November 2016
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	accepted calculation method
Justification for type of information:	Guidance on registration Reference: ECHA-16-G-06-EN Publ.date:November 2016 Practical guide 2: How to report weight of evidence - Reference: ECHA-10-B-05-EN Publ.date: 24/03/2010 "Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals" (ECHA 2008)
Reason / purpose for cross-reference:	other: weight of evidence
Reason / purpose for cross-reference:	other: weight of evidence
Reason / purpose for cross-reference:	other: weight of evidence
Qualifier:	according to guideline
Guideline:	other: REACH Guidance on Qsars and grouping of chemicals R.6 year 2008
Principles of method if other than guideline:	Consensus method: The predicted toxicity is estimated by taking an average of the predicted toxicities from the below QSAR methods (provided the predictions are within the respective applicability domains): Hierarchical method: The toxicity for a given query compound is estimated using the weighted average of the predictions from several different models. The different models are obtained by using Ward's method to divide the training set into a series of structurally similar clusters. A genetic algorithm based technique is used to generate models for each cluster. The models are generated prior to runtime. FDA method: The prediction for each test chemical is made using a new model that is fit to the chemicals that are most similar to the test compound. Each model is generated at runtime. Single model method: Predictions are made using a multilinear regression model that is fit to the training set (using molecular descriptors as independent variables) using a genetic algorithm based approach. The regression model is generated prior to runtime. Group contribution method: Predictions are made using a multilinear regression model that is fit to the training set (using molecular fragment counts as independent variables). The regression model is generated prior to runtime. Nearest neighbor method: The predicted toxicity is estimated by taking an average of the 3 chemicals in the training set that are most similar to the test chemical. User's Guide for T.E.S.T.(Toxicity Estimation Software Tool) T. Martin - U.S. EPA/National Risk Management Research Laboratory/Sustainable Technology Division, Cincinnati, OH 45268
Specific details on test material used for the study:	SMILES STRING CCCCCCCCC=CCCCCCCCC(=O)OCC(CC)(CO)CO
	Key result
Dose descriptor:	LD50
Effect level:	ca. 17 577 other: mg/kg
Conclusions:	Oral rat LD50 mg/kg 17577,74

Cross-reference 3

Reason / purpose for cross-reference:	other: weight of evidence

Reference

Endpoint:	acute toxicity: oral
Type of information:	other: data sharing dispute
Adequacy of study:	key study
Study period:	21 Juni - 05 July 1989
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	other: Guideline study without detailed restrictions Limited data on test substance
Justification for type of information:	Guidance on registration Reference: ECHA-16-G-06-EN Publ.date:November 2016 Practical guide 2: How to report weight of evidence - Reference: ECHA-10-B-05-EN Publ.date: 24/03/2010 "Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals" (ECHA 2008) According to Article 13 of Regulation (EC) No. 1907/2006 "General Requirements for Generation of Information on Intrinsic Properties of substances", information on intrinsic properties of substances may be generated by means other than tests e.g. from information from structurally related substances (grouping or read-across), provided that conditions set out in Annex XI are met. Annex XI, "General rules for adaptation of this standard testing regime set out in Annexes VII to X" states that "substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity may be considered as a group, or 'category' of substances. This avoids the need to test every substance for every endpoint".Since the category concept is applied to the polyol esters, data gaps will be filled by interpolation, as part of a read across approach from a representative category member(s) to avoid unnecessary animal testing. Additionally, once the category concept is applied, substances will be classified and labelled on this basis.Therefore, based on the group concept, all available data on repeated dose toxicity do not meet the classification criteria according to Regulation. See Category Justification Document Point enclosed at 13.2
Reason / purpose for cross-reference:	other: weight of evidence
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Reason / purpose for cross-reference:	other: weight of evidence
Qualifier:	equivalent or similar to guideline
Guideline:	EU Method B.1 (Acute Toxicity (Oral))
Version / remarks:	Limited data on test substance
Deviations:	yes
Remarks:	Limited data on test substance
GLP compliance:	yes
Test type:	standard acute method
Limit test:	yes
Specific details on test material used for the study:	- Name of test material (as cited in study report): only trade name given - Physical state: solid, white - Analytical purity: not reported
Species:	rat
Strain:	Wistar
Sex:	male/female
Details on test animals or test system and environmental conditions:	TEST ANIMALS - Source: Winkelmann, Borchen - Weight at study initiation: 187 g (male mean) and 167 g (female mean) - Fasting period before study: the animals were fasted 16 prior to 3 h after administration - Housing: Makrolon 3 - Diet: Altromin 1324, ad libitum - Water: tap water, ad libitum

	- Acclimation period: 7-8 days ENVIRONMENTAL CONDITIONS - Temperature (°C): 20-25 - Humidity (%): 45-60 - Photoperiod (hrs dark / hrs light): 12 / 12
Route of administration:	oral: gavage
Vehicle:	arachis oil
Details on oral exposure:	VEHICLE - Concentration in vehicle: 20% - Amount of vehicle (if gavage): 10 mL/kg
Doses:	2000 mg/kg bw
No. of animals per sex per dose:	5
Control animals:	other: not required
Details on study design:	- Duration of observation period following administration: 14 days - Frequency of observations and weighing: observations were done repeatedly on day of application, later on twice daily. Weighing on days -1, 2, 7 and 14 after application. - Necropsy of survivors performed: yes - Other examinations performed: gross pathology
Sex:	male/female
Dose descriptor:	LD50
Effect level:	> 2 000 mg/kg bw
Based on:	test mat.
Mortality:	No mortality occurred during this period.
Clinical signs:	other: No clinical signs of toxicity were observed up to the end of the 14-day observation period.
Gross pathology:	1 male animal with filled urinary bladder (not substance specific) was observed.
Interpretation of results:	GHS criteria not met
Remarks:	Migrated information Criteria used for interpretation of results: EU
Conclusions:	CLP: not classified DSD: not classified

Data source

Reference

Reference Type:	study report
Title:	Unnamed
Year:	2002
Report date:	2002

Materials and methods

Test guideline

Test guideline 1

Qualifier:	equivalent or similar to guideline
Guideline:	OECD Guideline 423 (Acute Oral toxicity - Acute Toxic Class Method)
Version / remarks:	adopted in 1996
Deviations:	yes
Remarks:	no analytical purity reported

Test guideline 2

Qualifier:	equivalent or similar to guideline
Guideline:	EU Method B.1 tris (Acute Oral Toxicity - Acute Toxic Class Method)
Version / remarks:	adopted in 1996
Deviations:	yes
Remarks:	no analytical purity reported

GLP compliance:	yes
Remarks:	Department of health of the government of the United Kingdom, UK
Test type:	acute toxic class method
Limit test:	yes

Test material

Test material information

Constituent 1

Reference substance name:	Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol
EC Number:	272-469-1
EC Name:	Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol
Cas Number:	68855-18-5
IUPAC Name:	68855-18-5

Specific details on test material used for the study:	- Name of test material (as cited in study report): only trade name given - Physical state: dark amber slightly viscous liquid - Analytical purity: no data - Storage condition of test material: room temperature in the dark

Results and discussion

Effect levels

Sex:	male/female
Dose descriptor:	LD50
Effect level:	> 2 000 mg/kg bw
Based on:	test mat.

Mortality:	No mortality occurred during the study period.
Clinical signs:	other: No clinical signs of toxicity were observed up to the end of the 14-day observation period.
Gross pathology:	Necropsy examination revealed no substance-related findings.

Applicant's summary and conclusion

Interpretation of results:	GHS criteria not met
Conclusions:	CLP: not classified