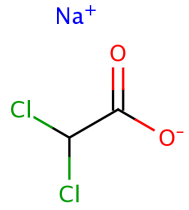
Chemical Summary: SODIUM DICHLOROACETATE (2156-56-1)

ACToR: Aggregated Computational Toxicology Resource

ACToR Database: actor_2015q1

ToxRefDB Database: toxrefdb_2010q1b



GCID	153827
MESH DESCRIPTION	
CASRN	2156-56-1
FORMULA	C2 H Cl2 Na O2
MW	150.9239
SMILES	O=C(C(Cl)Cl)[O-].[Na+]
SOURCE	DSSTox_prelim

Synonyms

2156-56-1

Acetic acid, dichloro-, sodium salt

Acetic acid, dichloro-, sodium salt

EINECS 218-461-3

Sodium dichloracetate

Sodium dichloroacetate

Toxicology Data

Hazard

NLM TOXNET CCRIS URL

Result group:

Component Name	Value
URL	*External Link*

NLM TOXNET CCRIS Data MSTU - MUTAGENICITY STUDIES

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA98
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA100
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1535
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1537
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA98
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA100
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1535
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1537
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	WP2 UVRA
Test System	E. COLI

Result group:

Component Name	Value
Dose Range	125-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	SUSPENSION/PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	L5187Y (TK+/TK-)
Test System	MOUSE LYMPHOMA

Result group:

Component Name	Value
Dose Range	125-5000 UG/ML
Metabolic Activation	NONE
Method	SUSPENSION/PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	L5178Y (TK+/TK-)
Test System	MOUSE LYMPHOMA

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	WP2 UVRA
Test System	E. COLI

Result group:

Component Name	Value
Dose Range	1-1000 UG/PLATE (TEST MATERIAL SOLVENT:DISTILLED WATER)
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[MEIER,JR, STEWART,BE AND BLAZAK,WF; GENOTOXICITY STUDIES OF SODIUM DICHLOROACETATE AND SODIUM TRICHLOROACETATE; ENVIRON. SCI. 5(2):95-108, 1997]

Results	NEGATIVE
Strain/Indicator	TA102
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	1-1000 UG/PLATE (TEST MATERIAL SOLVENT:DISTILLED WATER)
Metabolic Activation	RAT LIVER S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[MEIER,JR, STEWART,BE AND BLAZAK,WF; GENOTOXICITY STUDIES OF SODIUM DICHLOROACETATE AND SODIUM TRICHLOROACETATE; ENVIRON. SCI. 5(2):95-108, 1997]
Results	NEGATIVE
Strain/Indicator	TA102
Test System	AMES SALMONELLA TYPHIMURIUM

NLM TOXNET Toxicology

Result group:

Component Name	Value
Organism	mouse
PubMed ID	0
Reference	Journal of Agricultural and Food Chemistry. Vol. 10, Pg. 370, 1962.
Reported Dose	> 3gm/kg (3000mg/kg)
Test type	LD50

Result group:

Component Name	Value
Organism	mouse
PubMed ID	7097569
Reference	Journal of Pharmacology and Experimental Therapeutics. Vol. 222, Pg. 501, 1982.
Reported Dose	4845mg/kg (4845mg/kg)
Test type	LD50

Result group:

Component Name	Value
Organism	rat
PubMed ID	0
Reference	Journal of Industrial Hygiene and Toxicology. Vol. 23, Pg. 78, 1941.
Reported Dose	5281mg/kg (5281mg/kg)
Test type	LD50

Carcinogenicity

NLM TOXNET CCRIS URL

Result group:

Component Name	Value
URL	*External Link*

Genotoxicity

NLM TOXNET CCRIS Data MSTU - MUTAGENICITY STUDIES

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA98
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA100
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1535
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE

Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1537
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA98
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA100
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1535
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	TA1537
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	WP2 UVRA
Test System	E. COLI

Result group:

Component Name	Value
Dose Range	125-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	SUSPENSION/PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	L5187Y (TK+/TK-)
Test System	MOUSE LYMPHOMA

Result group:

Component Name	Value
Dose Range	125-5000 UG/ML
Metabolic Activation	NONE
Method	SUSPENSION/PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	L5178Y (TK+/TK-)
Test System	MOUSE LYMPHOMA

Result group:

Component Name	Value
Dose Range	333-5000 UG/PLATE
Metabolic Activation	RAT, LIVER, S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[FOX,AW, YANG,X, MURLI,H, LAWLOR,TE, CIFONE,MA AND RENO,FE; ABSENCE OF MUTAGENIC EFFECTS OF SODIUM DICHLOROACETATE; FUNDAM. APPL. TOXICOL. 32(1):87-95, 1996]
Results	NEGATIVE
Strain/Indicator	WP2 UVRA
Test System	E. COLI

Result group:

Component Name	Value
Dose Range	1-1000 UG/PLATE (TEST MATERIAL SOLVENT:DISTILLED WATER)
Metabolic Activation	NONE
Method	STANDARD PLATE
Reference	[MEIER,JR, STEWART,BE AND BLAZAK,WF; GENOTOXICITY STUDIES OF SODIUM DICHLOROACETATE AND SODIUM TRICHLOROACETATE; ENVIRON. SCI. 5(2):95-108, 1997]
Results	NEGATIVE
Strain/Indicator	TA102
Test System	AMES SALMONELLA TYPHIMURIUM

Result group:

Component Name	Value
Dose Range	1-1000 UG/PLATE (TEST MATERIAL SOLVENT:DISTILLED WATER)
Metabolic Activation	RAT LIVER S-9, AROCLOR 1254
Method	STANDARD PLATE
Reference	[MEIER,JR, STEWART,BE AND BLAZAK,WF; GENOTOXICITY STUDIES OF SODIUM DICHLOROACETATE AND SODIUM TRICHLOROACETATE; ENVIRON. SCI. 5(2):95-108, 1997]
Results	NEGATIVE
Strain/Indicator	TA102
Test System	AMES SALMONELLA TYPHIMURIUM

Non-regulatory Risk Management

Total Use, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Industrial use, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Specialized construction activities

Exposure, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Air	x = One or several uses indicate a potential exposure
Consumer	xx: One or several uses indicate a probable exposure
Country	Sweden
Range_of_use	x = One or several uses indicate a potential exposure
Surface_Water	- The registered uses do not indicate direct exposure, but use categories do not include all potential uses of the chemical and possibility for direct exposure cannot be excluded.
Waste_Water	- The registered uses do not indicate direct exposure, but use categories do not include all potential uses of the chemical and possibility for direct exposure cannot be excluded.

Result group:

Component Name	Value
Air	x = One or several uses indicate a potential exposure
Consumer	x = One or several uses indicate a potential exposure
Country	Norway
Range_of_use	xx: One or several uses indicate a probable exposure
Surface_Water	xx: One or several uses indicate a probable exposure
Waste_Water	xx: One or several uses indicate a probable exposure

Use by Category, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Denmark
Use	Lubricants and Other Additives

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Sweden
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Denmark
Use	Lubricants and Other Additives

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Finland
Use	Coloring agents

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Detailed Use by Category, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	N
DetailedUse	Paint lacquers and varnishes

Regulatory Risk Management

China Chemical Inventory

Result group:

Component Name	Value
Chinese name	...'
English Alias	Dichloroacetic acid sodium salt
Formula	C2H2Cl2O2Na

FDA Drugs with Orphan Status

Result group:

Component Name	Value
Contact Company	Stacpoole, Peter W. M.D., Ph.D.
Contact company address	University of Florida
Contact company address	P.O. Box 100277
Contact company City	Gainesville
Contact company country	UNITED STATES
Contact company State	FL
Contact company zip code	32610
Designated Date	33035
Designated Indication	Treatment of congenital lactic acidosis
Orphan drug status	Designated

Result group:

Component Name	Value
Contact Company	Stacpoole, Peter W. M.D., Ph.D.
Contact company address	University of Florida
Contact company address	P.O. Box 100277
Contact company City	Gainesville
Contact company country	UNITED STATES
Contact company State	FL
Contact company zip code	32610
Designated Date	33035
Designated Indication	Treatment of homozygous familial hypercholesterolemia.
Orphan drug status	Designated

Result group:

Component Name	Value
Contact Company	Stacpoole, Peter W. M.D., Ph.D.
Contact company address	University Of Florida
Contact company address	P.O. Box 100277
Contact company City	Gainesville

Contact company country	UNITED STATES
Contact company State	FL
Contact company zip code	32610
Designated Date	34648
Designated Indication	Treatment of lactic acidosis in patients with severe malaria.
Orphan drug status	Designated

Result group:

Component Name	Value
Contact Company	Questcor Pharmaceuticals, Inc.
Contact company address	3260 Whipple Rd.
Contact company City	Union City
Contact company country	UNITED STATES
Contact company State	CA
Contact company zip code	94587-1217
Designated Date	35795
Designated Indication	Treatment of congenital lactic acidosis.
Orphan drug status	Designated/Withdrawn

Result group:

Component Name	Value
Contact Company	Questcor Pharmaceuticals, Inc.
Contact company address	3260 Whipple Rd.
Contact company City	Union City
Contact company country	UNITED STATES
Contact company State	CA
Contact company zip code	94587-0700
Designated Date	36325
Designated Indication	Treatment of severe head injury.
Orphan drug status	Designated/Withdrawn
Trade name	Ceresine

Result group:

Component Name	Value
Contact Company	EBD Group
Contact company address	2032 Corte del Nogal
Contact company address	Suite 120
Contact company City	Carlsbad
Contact company country	UNITED STATES
Contact company State	CA
Contact company zip code	92011
Designated Date	37805
Designated Indication	Use as an antidote in the management of systemic monochloroacetic acid poisoning
Orphan drug status	Designated

Result group:

Component Name	Value
Contact Company	Peter W. Stackpoole, PhD, MD
Contact company address	University of FL College of Medicine
Contact company address	P. O. Box 100226
Contact company City	Gainesville
Contact company country	UNITED STATES
Contact company State	FL
Contact company zip code	32611
Designated Date	40511
Designated Indication	For pulmonary arterial hypertension.
Orphan drug status	Designated

SRS -- EPA Substance Regulatory Services List

Result group:

Component Name	Value
TSCATS -- Toxic Substances Control Act Test Submissions	Subject to specified regulation

Production and Release

EDSPDB Production/Import Volumes

Result group:

Component Name	Value
AIRHALF	352
BCF	3.161999941
BCF_Rank	61277
BCF_Source	Predicted - SRC BCF
H2OHALF	360
PERSIST	345
SEDHALF	1440
SOILHALF	360

Total Use, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Industrial use, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Specialized construction activities

Exposure, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Air	x = One or several uses indicate a potential exposure
Consumer	xx: One or several uses indicate a probable exposure
Country	Sweden
Range_of_use	x = One or several uses indicate a potential exposure
Surface_Water	- The registered uses do not indicate direct exposure, but use categories do not include all potential uses of the chemical and possibility for direct exposure cannot be excluded.
Waste_Water	- The registered uses do not indicate direct exposure, but use categories do not include all potential uses of the chemical and possibility for direct exposure cannot be excluded.

Result group:

Component Name	Value
Air	x = One or several uses indicate a potential exposure
Consumer	x = One or several uses indicate a potential exposure
Country	Norway
Range_of_use	xx: One or several uses indicate a probable exposure
Surface_Water	xx: One or several uses indicate a probable exposure
Waste_Water	xx: One or several uses indicate a probable exposure

Use by Category, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Denmark
Use	Lubricants and Other Additives

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Sweden
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Denmark
Use	Lubricants and Other Additives

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Finland
Use	Coloring agents

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Detailed Use by Category, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	N

DetailedUse	Paint lacquers and varnishes

In Vitro

DSSTox ArrayExpress DSSTox Annotation

Result group:

Component Name	Value
Chemical StudyType	Treatment
Experiment Accession	E-GEOD-6014
Experiment URL	*External Link*
Study Type	microarray

DSSTox GEO DSSTox Annotation

Result group:

Component Name	Value
Chemical StudyType	Combination_TreatmentANDTreatment
Experiment Accession	GSE6014
Experiment URL	*External Link*
Study Type	microarray

Inherent Chemical Property

ChEMBL chemical property data

Result group:

Component Name	Value
Medicinal Chemistry Friendly?	Y
molecular species	ACID
Number of Rule of 5 Violations	0
Pass rule of 3	Y

Environmental Releases from EDSPDB

Result group:

Component Name	Value
AIRHALF	345
BCF_Rank	3.161999941
BCF_Source	61277
H2OHALF	352
PERSIST	Predicted - SRC BCF
PERS_Rank	1440
SEDHALF	360
SOILHALF	360

Use

ChEMBL chemical property data

Result group:

Component Name	Value
Medicinal Chemistry Friendly?	Y
molecular species	ACID
Number of Rule of 5 Violations	0
Pass rule of 3	Y

ChEMBL activity data

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Binding
Curation	Expert
Description	Inhibitory activity tested against Pyruvate Dehydrogenase Kinase (PDHK) receptor from rats.
Operator	>
Organism	Rattus norvegicus
Reference	J. Med. Chem. (2000) 2:236-249
Target	Pyruvate dehydrogenase kinase isoform 1
Target Mapping	Multiple homologous proteins
Units	nM

Result group:

Component Name	Value
Activity Type	EC50
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Intermediate
Description	Effective concentration required to increase the oxidation of lactate in cellular assay using Human Skin Fibroblasts
Operator	=
Organism	Homo sapiens
Reference	J. Med. Chem. (2000) 2:236-249
Target	Homo sapiens
Target Mapping	Non-molecular
Units	nM

Result group:

Component Name	Value
Activity Type	Control
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Intermediate

Description	In vivo %control of lactate in normal Sprague-Dawley rats after 2 hr at a dose of 1 umol/Kg
Operator	=
Organism	Rattus norvegicus
Reference	J. Med. Chem. (2000) 2:236-249
Target	Rattus norvegicus
Target Mapping	Non-molecular
Units	%

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Binding
Curation	Expert
Description	Inhibitory activity against Pyruvate dehydrogenase kinase
Operator	>
Organism	Homo sapiens
Reference	J. Med. Chem. (1999) 15:2741-2746
Target	Pyruvate dehydrogenase kinase isoform 2
Target Mapping	Multiple homologous proteins
Units	nM

Result group:

Component Name	Value
Activity Type	EC50
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Expert
Description	In vivo inhibion of pyruvate dehydrogenase kinase, increased oxidation of lactate
Operator	=
Organism	Homo sapiens
Reference	J. Med. Chem. (1999) 15:2741-2746
Target	Pyruvate dehydrogenase kinase isoform 2
Target Mapping	Multiple proteins
Units	nM

Result group:

Component Name	Value
Activity Type	Control
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Expert
Description	In vivo inhibition of pyruvate dehydrogenase kinase, reduced lactate level in normal 24 hr r fasted rats at 1 mmol/kg oral dose
Operator	=
Organism	Rattus norvegicus
Reference	J. Med. Chem. (1999) 15:2741-2746
Target	Pyruvate dehydrogenase kinase isoform 1
Target Mapping	Multiple proteins
Units	%

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Binding
Curation	Expert
Description	Inhibition of porcine pyruvate dehydrogenase kinase (PDHK)in a primary enzymatic assay
Operator	>
Organism	Homo sapiens
Reference	J. Med. Chem. (2000) 11:2248-2257
Target	Pyruvate dehydrogenase kinase isoform 2
Target Mapping	Multiple homologous proteins
Units	nM

Result group:

Component Name	Value
Activity Type	EC50
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Intermediate
Description	Effective concentration in human fibroblasts for increased oxidation of lactate
Operator	=
Organism	Homo sapiens
Reference	J. Med. Chem. (2000) 11:2248-2257
Target	Homo sapiens
Target Mapping	Non-molecular
Units	nM

Result group:

Component Name	Value
Activity Type	Control

Assay Source	Scientific Literature
Assay Type	Functional
Curation	Expert
Description	In vivo percent of control lactate in 24 hr fasted rats at 1 mM/kg oral dose
Operator	=
Organism	Rattus norvegicus
Reference	J. Med. Chem. (2000) 11:2248-2257
Target	Pyruvate dehydrogenase kinase isoform 1
Target Mapping	Multiple proteins
Units	%

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Autocuration
Description	Anticancer activity against human BGC823 cells after 72 hrs by MTT assay
Operator	=
Reference	Eur. J. Med. Chem. (2010) 9:4300-4306
Target Mapping	Unassigned
Units	nM

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Functional
Cell Line	KB
Curation	Autocuration
Description	Anticancer activity against human KB cells after 72 hrs by MTT assay
Operator	=
Organism	Homo sapiens
Reference	Eur. J. Med. Chem. (2010) 9:4300-4306
Target	KB (Squamous cell carcinoma)
Target Mapping	Non-molecular
Units	nM

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Functional
Cell Line	A549
Curation	Autocuration
Description	Anticancer activity against human A549 cells after 72 hrs by MTT assay
Operator	=
Organism	Homo sapiens
Reference	Eur. J. Med. Chem. (2010) 9:4300-4306
Target	A549 (Lung carcinoma cells)
Target Mapping	Non-molecular
Units	nM

Result group:

Component Name	Value
Activity Type	IC50
Assay Source	Scientific Literature
Assay Type	Functional
Curation	Autocuration
Description	Anticancer activity against human Bel7402 cells after 72 hrs by MTT assay
Operator	=
Reference	Eur. J. Med. Chem. (2010) 9:4300-4306
Target Mapping	Unassigned
Units	nM

Total Use, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Result group:

Component Name	Value
Country	Norway

Industrial use, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Construction

Result group:

Component Name	Value
Country	Norway
Use	Specialized construction activities

Exposure, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Air	x = One or several uses indicate a potential exposure
Consumer	xx: One or several uses indicate a probable exposure
Country	Sweden
Range_of_use	x = One or several uses indicate a potential exposure
Surface_Water	- The registered uses do not indicate direct exposure, but use categories do not include all potential uses of the chemical and possibility for direct exposure cannot be excluded.
Waste_Water	- The registered uses do not indicate direct exposure, but use categories do not include all potential uses of the chemical and possibility for direct exposure cannot be excluded.

Result group:

Component Name	Value
Air	x = One or several uses indicate a potential exposure
Consumer	x = One or several uses indicate a potential exposure
Country	Norway
Range_of_use	xx: One or several uses indicate a probable exposure
Surface_Water	xx: One or several uses indicate a probable exposure
Waste_Water	xx: One or several uses indicate a probable exposure

Use by Category, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Denmark
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Denmark
Use	Lubricants and Other Additives

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Sweden
Use	Adhesives and binding agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Result group:

Component Name	Value
Country	Denmark
Use	Lubricants and Other Additives

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Finland
Use	Coloring agents

Result group:

Component Name	Value
Country	Sweden
Use	Reprographic agents

Result group:

Component Name	Value
Country	Norway
Use	Paints lacquers and varnishes

Detailed Use by Category, Substances in Preparations in Nordic Countries

Result group:

Component Name	Value
Country	N
DetailedUse	Paint lacquers and varnishes
Data Collection	**Note**

External Searches by Name or CAS

TOXNET CCRIS
TOXNET DART ETIC
TOXNET EMIC
TOXNET GENETOX
TOXNET HazMap
TOXNET Houshold Products

TOXNET HSDB
TOXNET MESH Headings
TOXNET TOXLINE
TOXNET TOXMAP
ChemIDPlus Advanced
PubMed Cancer
PubMed Toxicology
NIST Chemistry Webbook
NTP Study Search
EPA Substance Registry System (EPA SRS)