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# I U C L I D

## Data Set

# Robust Summaries

**Existing Chemical** : ID: 4131-74-2  
**CAS No.** : 4131-74-2  
**EINECS Name** : dimethyl 3,3'-thiobispropionate  
**EC No.** : 223-948-9  
**Molecular Formula** : C<sub>8</sub>H<sub>14</sub>O<sub>4</sub>S

**Status** :  
**Memo** : Mark 5152 US HPV Crompton Corporation

**Printing date** : 25.06.2003  
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**Number of pages** : 24

**Chapter (profile)** : Chapter: 2, 3, 4, 9  
**Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4  
**Flags (profile)** : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),  
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 2. Physico-Chemical Data

Id 4131-74-2  
Date 08.05.2003

### 2.1 MELTING POINT

Value : -38.3 °C  
Sublimation :  
Method : other: Estimation using MPBPWIN v1.40  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
Remark : Substance is a liquid at room temperature.  
Reliability : (2) valid with restrictions  
27.03.2003 (9)

### 2.2 BOILING POINT

Value : 148°C at 18 mm Hg  
Decomposition :  
Method : Literature  
Year : 2004  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
Result : 148 C at 18 mmHga  
161-162 C at 18 mmHgb  
162-164 C at 18 mmHgb, d  
158-159 C at 10 mmHgb  
148.5-149 C at 8 mmHgb  
138-139 C at 6 mmHgb,d  
130 C at 2 mmHgc  
Reliability : (2) valid with restrictions  
01.03.2004 (10)(11)(12)(13)(14)

### 2.4 VAPOUR PRESSURE

Value : .055 hPa at 25 °C  
Decomposition :  
Method : other (calculated): MPBPWIN v1.40  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
Reliability : (2) valid with restrictions  
27.03.2003 (9)

### 2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water  
Log pow : .98 at °C  
pH value :  
Method : other (calculated): KOWWIN v1.66  
Year : 2003  
GLP :

## 2. Physico-Chemical Data

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**Test substance** : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
**Reliability** : (2) valid with restrictions  
27.03.2003 (9)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water  
**Description** : not soluble  
**Method** : other: unknown  
**Year** : 2002  
**GLP** : no data  
**Test substance** : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
**Reliability** : (4) not assignable  
08.05.2003 (2)

### 3. Environmental Fate and Pathways

Id 4131-74-2  
Date 08.05.2003

#### 3.1.1 PHOTODEGRADATION

Type : air  
Light source :  
Light spectrum : nm  
Relative intensity : based on intensity of sunlight  
**DIRECT PHOTOLYSIS**  
Halflife t1/2 : 6.2 hour(s)  
Degradation : % after  
Quantum yield :  
Deg. product :  
Method : other (calculated): AOPWIN v1.90  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
  
Remark : Concentration of hydroxyl radicals in air = 1.5E6 OH/cm3  
12-hour day  
27.03.2003 (9)

#### 3.1.2 STABILITY IN WATER

Type : abiotic  
t1/2 pH4 : at °C  
t1/2 pH7 : at °C  
t1/2 pH9 : at °C  
Deg. product :  
Method : other (calculated): Estimated using HYDROWIN v1.67  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
  
Result : Half life at pH 8: 37.14 days  
Half life at pH 7: 1.02 years  
Reliability : (2) valid with restrictions  
27.03.2003 (9)

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III  
Media :  
Air : % (Fugacity Model Level I)  
Water : % (Fugacity Model Level I)  
Soil : % (Fugacity Model Level I)  
Biota : % (Fugacity Model Level II/III)  
Soil : % (Fugacity Model Level II/III)  
Method : other: Calculation using EPIWIN Level III Fugacity Model  
Year : 2003

### 3. Environmental Fate and Pathways

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**Test condition** : Henry's Law Constant: 3.15E-10 atm-m<sup>3</sup>/mole (Henrywin program)  
 Vapor pressure: 0.0417 mmHg (Mpbpwin program)  
 Log Kow: 0.98 (experimental value)  
 Soil Koc: 3.92 (calc by model)

1000 kg/hr emissions to air, water and soil compartments.  
**Test substance** : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	0.01	12.4	1000
Water	42	360	1000
Soil	57.9	360	1000
Sediment	0.0757	1.44E+3	0

  

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.51E-13	7.17	1.28	0.239	0.0426
Water	4.09E-15	1.03E+3	536	34.4	17.9
Soil	1.59E-13	1.42E+3	0	47.4	0
Sediment	3.37E-15	0.465	0.0193	0.0155	0.000645

Persistence time: 425 hr  
 Reaction time: 518 hr  
 Advection time: 2.38E+3 hr  
 Percent reacted: 82.1  
 Percent advected: 17.9

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):

Air: 12.36  
 Water: 360  
 Soil: 360  
 Sediment: 1440  
 Biowin estimate: 3.024 (weeks)

Advection times (hr):

Air: 100  
 Water: 1000  
 Sediment: 5E+4

**Reliability** : (1) valid without restriction  
 27.03.2003

(9)

#### 3.5 BIODEGRADATION

**Type** : Aerobic  
**Inoculum** :  
**Deg. product** :  
**Method** : other: estimation using BIOWIN v4.00  
**Year** : 2003  
**GLP** :  
**Test substance** : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)

### 3. Environmental Fate and Pathways

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**Result** : MITI Linear Biodegradation Probability = 0.9845  
MITI Non-linear Biodegradation Probability = 0.9616

**Reliability** : The substance is predicted to be readily biodegradable  
27.03.2003 : (2) valid with restrictions

(9)

**4.1 ACUTE/PROLONGED TOXICITY TO FISH**

Type :  
Species :  
Exposure period : 96 hour(s)  
Unit : mg/l  
LC50 : 109.7  
Method : other: Estimated using ECOSAR v0.99g  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
Test condition : Log Kow: 0.98 (KOWWIN estimate)  
Water solubility: 1E+4 mg/l  
Ecosar Class: Esters  
Reliability : (2) valid with restrictions  
27.03.2003 (9)

**4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES**

Type :  
Species : Daphnia sp. (Crustacea)  
Exposure period : 48 hour(s)  
Unit : mg/l  
EC50 : 1388.7  
Method : other: Estimated using ECOSAR v0.99g  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
Test condition : Log Kow: 0.98 (KOWWIN estimate)  
Water solubility: 1E+4 mg/l  
Ecosar Class: Esters  
Reliability : (2) valid with restrictions  
27.03.2003 (9)

**4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE**

Species :  
Endpoint :  
Exposure period : 96 hour(s)  
Unit : mg/l  
EC50 : 8.41  
Method : other: Estimated using ECOSAR v0.99g  
Year : 2003  
GLP :  
Test substance : Propanoic acid, 3,3'-thiobis-, dimethyl ester (CAS No. 4131-74-2)  
Test condition : Log Kow: 0.98 (KOWWIN estimate)  
Water solubility: 1E+4 mg/l  
Ecosar Class: Esters  
Reliability : (2) valid with restrictions

27.03.2003

(9)

**5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**

**In Vitro/in vivo** : In vivo  
**Type** :  
**Species** : rat  
**Number of animals**  
     **Males** :  
     **Females** :  
**Doses**  
     **Males** :  
     **Females** :  
**Vehicle** :  
**Method** :  
**Year** : 1973  
**GLP** : no  
**Test substance** : Thiodipropionic acid (CAS No. 111-17-1)  
     Didodecyl thiodipropionate (CAS No. 123-28-4)  
     POLY-TDPS-2000

[1-<sup>14</sup>C]Thiodipropionic acid ([<sup>14</sup>C]TDPA) of specific activity 1.71 mCi/mmol was used to prepare <sup>14</sup>C-labeled POLY\_TDPS-2000 ([<sup>14</sup>C]TDPS) of specific activity 5 μCi/mg (equivalent to 58% TDPA).

Carboxy <sup>14</sup>C-labeled didocyl thiodipropionate ([<sup>14</sup>C]DDTDP), specific activity 60 μCi/mmol. was purified (99.2%) by recrystallization from aqueous acetone.

**Method** : Animals: Male Sprague-Dawley rats weighing 215-325 g were housed in glass metabolism chambers fitted for the collection of urine, feces and respiratory CO<sub>2</sub>.

Dosages: In some experiments the dose was incorporated into feed. Starved rats were given the food and CO<sub>2</sub> collection was started. After 4-8 hr any unconsumed dose was removed and rats were returned to the regular diet.

In other experiments the dissolved dose was intubated in to the stomach. [<sup>14</sup>C]TDPA was dissolved in ethanol-water (1:1) and [<sup>14</sup>C]DDTDP in corn oil.

Urines and feces in the [<sup>14</sup>C]TDPS study were collected at the end of dosing and then at 24 hr intervals. [<sup>14</sup>C]TDPA and [<sup>14</sup>C]DDTDP experiment urines and CO<sub>2</sub> absorbers were processed daily. Liver, kidneys, brain, heart, lungs, whole gastrointestinal tracts and fat samples were removed at sacrifice and frozen with carcasses until assayed.

**Result** : Elimination of radioactivity:

[<sup>14</sup>C]TDPA and [<sup>14</sup>C]TDPS were almost entirely absorbed from the gastrointestinal tract when fed at levels of 3-6 mg/kg, and [<sup>14</sup>C]TDPA and [<sup>14</sup>C]DDTDP were almost entirely absorbed at levels up to 650 and 210

mg/kg, respectively (Table 1). Urinary excretion represented the major pathway of disposal for all 3 materials, generally accounting for 90% of the total eliminate in all experiments. Elimination of radioactivity as  $^{14}\text{CO}_2$  was significant in all experiments, amounting to about 5% of the dose. Elimination was very rapid. Over 90% of the total radioactivity eliminated was eliminated in less than 24 hour by all rats (Table 2). The excretion patterns and rates did not appear to be dose-related (Table 1).

Distribution of radioactivity in organs at sacrifice:

Levels of radioactivity of organs from rats fed  $[^{14}\text{C}]\text{TDPS}$  were slightly elevated at 4 days but had decreased to normal by 34 days. The value in fat was somewhat higher than the other tissue values at 4 days but had decreased to the same levels as the other tissues by 34 days. Rats fed  $[^{14}\text{C}]\text{TDPA}$  and  $[^{14}\text{C}]\text{DDTDP}$  had tissue radioactivity values throughout which were close to normal values except that the value of radioactivity in the fat of rats fed  $[^{14}\text{C}]\text{DDTDP}$  were elevated at 4 days after dosing and remained so at 8 and 34 days.

Nature of the radioactive urinary metabolites of  $[^{14}\text{C}]\text{TDPA}$ ,  $[^{14}\text{C}]\text{TDPS}$  and  $[^{14}\text{C}]\text{DDTDP}$ :

Thin-layer and paper chromatography of urine for metabolite detection was unsuccessful because of the tendency of TDPA to migrate as more than one spot with most solvent systems. In consequence, reverse isotope dilution studies were carried out with untreated and hydrolyzed urines to assay elimination of free and combined  $[^{14}\text{C}]\text{TDPA}$  (Table 2). Acid hydrolyses were performed without added TDPA in the  $[^{14}\text{C}]\text{TDPS}$  studies, but after addition of TDPA in the  $[^{14}\text{C}]\text{TDPA}$  and  $[^{14}\text{C}]\text{DDTDP}$  experiments. Assays of untreated urines from rats fed  $[^{14}\text{C}]\text{TDPA}$  and  $[^{14}\text{C}]\text{TDPS}$  at low dose levels (3.1 and 5.6 mg/kg) showed only a small portion of the radioactivity was eliminated as free TDPA. At high dose levels (627 mg/kg), most of the excreted radioactivity was free TDPA. Acid hydrolysis of urine samples afforded high recovery of radioactivity as TDPA, approaching 10% of the urinary radioactivity after feeding  $[^{14}\text{C}]\text{TDPA}$  and  $[^{14}\text{C}]\text{DDTDP}$  and 70% after  $[^{14}\text{C}]\text{TDPS}$ .

To determine whether the combined radioactivity was present as an ester glucuronide, a urine sample from a rat fed  $[^{14}\text{C}]\text{TDPS}$  at the low level was hydrolyzed with  $\beta$ -glucuronidase.  $[^{14}\text{C}]\text{TDPA}$  amounted to 14.4% of the urinary radioactivity compared to 7.0% without treatment. Mild alkaline hydrolysis was unsuccessful and led to decomposition of TDPA.

The results show that oral doses of  $[^{14}\text{C}]\text{TDPA}$  in the range of 3-650 mg/kg are almost entirely and rapidly absorbed from the gastrointestinal tract of the rat, and that the absorbed  $[^{14}\text{C}]\text{TDPA}$  is very rapidly eliminated in the urine with only a small amount entering an oxidative metabolic pathway.

Reverse isotope dilution studies indicate that  $[^{14}\text{C}]\text{TDPA}$  is excreted in the urine either largely unchanged (627 mg/kg dose) or as an acid labile conjugate (3.1 mg/kg dose) which is apparently not a glucuronide.

The disposition of  $[^{14}\text{C}]\text{TDPA}$  combined as part of the TDPS or DDTDP molecules was very similar to the disposition of orally intubated free  $[^{14}\text{C}]\text{TDPA}$ . The rapidity of elimination, the relative importance of the

various pathways, and the tissue retentions for each substance were not apparently different. At least 65% of ingested [ $^{14}\text{C}$ ]TDPS appeared as free or combined [ $^{14}\text{C}$ ]TDPA in the urine, the metabolites apparently being identical with those found after feeding [ $^{14}\text{C}$ ]TDPA. Similarly, [ $^{14}\text{C}$ ]DDTDP was also excreted as free [ $^{14}\text{C}$ ]TDPA or an acid labile conjugate. The identification of only 65% of the urinary radioactivity in the [ $^{14}\text{C}$ ]TDPS study as free or combined [ $^{14}\text{C}$ ]TDPA could be due to degradation by the acid of the small quantities of [ $^{14}\text{C}$ ]TDPA present.

Tissue radioactivity levels indicate that large oral doses of [ $^{14}\text{C}$ ]TDPA lead neither to preferential incorporation of the label into tissues nor to a significant increase in the general tissue radioactivity.

Rats fed [ $^{14}\text{C}$ ]TDPS showed a slight initial increase in the level of radioactivity in most tissues and slightly larger incorporation into the fat. These levels declined to background values by day 34. This radioactivity could arise from TDPS partially absorbed as fat-soluble esters which may be widely disseminated but are fairly rapidly eliminated.

Feeding of large doses of DDTDP led to some retention of radioactivity by fat. This radioactivity still remained after 34 days.

The intake levels encountered in use at the maximum allowable daily intake would be markedly lower than the doses used in this study and it is expected that there would be rapid elimination of all these substances, probably as thiodipropionic acid and the constituent moieties, with negligible retention by the organism.

Table 1: Elimination of rats fed [ $^{14}\text{C}$ ]TDPA, [ $^{14}\text{C}$ ]DDTDP and [ $^{14}\text{C}$ ]TDPS

Compound	Rat No.	Method <sup>a</sup>	Dose			Time (days)	Elimination (% of dose)			
			mg	mg/kg	$\mu\text{Ci}$		Urine	$\text{CO}_2$	Feces	Totals
[ $^{14}\text{C}$ ]TDPA	1	Gavage	1.0	3.1	9.3	4	90.1	3.1	0.5	93.6
	2	Gavage	152	650	9.0	4	78.1	8.2	0.5	86.8
	3	Gavage	160	572	9.3	4	84.5	2.8	0.9	88.4
	4	Gavage	152	551	8.9	8	88.5	7.2	0.2	95.9
	5	Feed	55	241	8.2	34	87.4	3.3 <sup>a</sup>	0.1 <sup>b</sup>	90.7
[ $^{14}\text{C}$ ]DDTDP	1	Gavage	32	107	3.3	4	84.6	2.9	3.5	90.9
	2	Gavage	64	208	6.6	8	88.5	3.9	1.8	94.2
	3	Feed	36	166	4.0	34	86.1	3.2 <sup>a</sup>	0.1 <sup>b</sup>	89.4
[ $^{14}\text{C}$ ]TDPS	1	Feed	1.4	5.6	6.9	4	94.7	5.9	0.7	101.2
	2	Feed	1.3	4.8	6.2	8	95.4	5.3	0.6	101.3
	3	Feed	1.1	4.7	5.3	34	97.6	7.4 <sup>a</sup>	0.7 <sup>b</sup>	105.6

<sup>a</sup> By direct scintillation assay; others by  $\text{BaCO}_3$  procedure

<sup>b</sup> By hydrolysis and direct assay; others by extraction and combustion.

Table 2: Recovery of [ $^{14}\text{C}$ ]TDPA from rat urine by isotope dilution<sup>a</sup>

Material fed	Dose (mg/kg)	Treatment <sup>b</sup>	% of urine radioactivity <sup>c</sup>
[ $^{14}\text{C}$ ]TDPA	3.1	pH to 10 and then to <2	7.0 (2)
		Acid hydrolysis (3N) with added TDPA	104.6 (2)
	627	pH to 10 and then to <2	80.9 (2)
		Acid hydrolysis (3N) with added TDPA	107.3 (2)

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$^{14}\text{C}$ DDTDP	107	Acid hydrolysis (3N) with added TDPA	93.3 (3)
	208	Acid hydrolysis (3N) with added TDPA	100.0 (3)
	166	Acid hydrolysis (3N) with added TDPA	100.0 (3)
$^{14}\text{C}$ TDPS	5.6	None	3.5 (5)
		Acid hydrolysis (6N), no added TDPA	66.7 (3)

<sup>a</sup> TDPA and TDPS by Geiger counter, DDTDP by scintillation spectrometer. Each value is a single experiment

<sup>b</sup> None indicates addition of TDPA and recrystallization at pH 2

<sup>c</sup> Number in parentheses indicated number of recrystallizations

**Conclusion** : The results show that esters of TDPA are almost completely absorbed and hydrolyzed to TDPA, which is itself largely eliminated in the urine, either as the free acid or conjugated.

**Reliability** : (1) valid without restriction  
10.04.2003

(7)

### 5.1.1 ACUTE ORAL TOXICITY

**Type** : LD50  
**Value** : > 2500 mg/kg bw  
**Species** : rat  
**Strain** : no data  
**Sex** : no data  
**Number of animals** :  
**Vehicle** : other: olive oil  
**Doses** : 2000, 2500 mg/kg bw  
**Method** :  
**Year** : 1947  
**GLP** : no  
**Test substance** : Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4)  
Purity: >97% w/w

**Method** : Groups of 5 or 10 rats were dosed orally with 2000 or 2500 mg/kg, respectively. Test material was dissolved in olive oil. Dosed animals were observed for 7 days after dosing.

**Result** : There were no deaths observed at either dose level.

**Reliability** : (2) valid with restrictions

10.04.2003

(8)

**Type** : LD50  
**Value** : > 5000  
**Species** : rat  
**Strain** : no data  
**Sex** : male  
**Number of animals** :  
**Vehicle** : physiol. saline  
**Doses** : 50, 500, 5000 mg/kg bw  
**Method** :  
**Year** : 1973  
**GLP** : no

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<b>Test substance</b>	:	Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4) Purity: >97% w/w	
<b>Method</b>	:	A group of 12 male rats was dosed with 5000 mg/kg while groups of 10 male rats were dosed with 50 or 500 mg/kg. Animals were necropsied on day 6.	
<b>Result</b>	:	All animals survived to the scheduled necropsy and appeared normal during the 5 day observation period. No gross morphological changes were observed.	
<b>Reliability</b> 07.04.2003	:	(2) valid with restrictions	(6)
<b>Type</b>	:	LD50	
<b>Value</b>	:	> 2000 mg/kg bw	
<b>Species</b>	:	mouse	
<b>Strain</b>	:	no data	
<b>Sex</b>	:	no data	
<b>Number of animals</b>	:		
<b>Vehicle</b>	:	other: olive oil	
<b>Doses</b>	:	300, 500, 1000, 2000 mg/kg	
<b>Method</b>	:		
<b>Year</b>	:	1947	
<b>GLP</b>	:	no	
<b>Test substance</b>	:	Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4) Purity: >97% w/w	
<b>Method</b>	:	Groups of 19, 10, 20 or 20 mice were dosed orally with 300, 500, 1000 or 2000 mg/kg, respectively. Test material was dissolved in olive oil. Animals were observed for one week after dosing with the test material.	
<b>Result</b>	:	There were 4, 0, 0, 1 deaths observed at 300, 5000, 1000 and 2000 mg/kg, respectively.	
		No further information was provided.	
<b>Reliability</b> 07.04.2003	:	(2) valid with restrictions	(8)
<b>Type</b>	:	LD50	
<b>Value</b>	:	2000 mg/kg bw	
<b>Species</b>	:	mouse	
<b>Strain</b>	:		
<b>Sex</b>	:		
<b>Number of animals</b>	:		
<b>Vehicle</b>	:		
<b>Doses</b>	:		
<b>Method</b>	:		
<b>Year</b>	:	1951	
<b>GLP</b>	:		
<b>Test substance</b>	:	Thiodipropionic acid (CAS No. 111-17-1) Purity: No data	
<b>Method</b>	:	No Experimental details available	
<b>Reliability</b> 11.04.2003	:	(4) not assignable	(5)

## 5. Toxicity

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Type : LD50  
Value : 3000 mg/kg bw  
Species : rat  
Strain :  
Sex :  
Number of animals :  
Vehicle :  
Doses :  
Method :  
Year : 1951  
GLP :  
Test substance : Thiodipropionic acid (CAS No. 111-17-1)  
Purity: No data

Method : No Experimental details available  
Reliability : (4) not assignable  
11.04.2003

(5)

### 5.4 REPEATED DOSE TOXICITY

Type :  
Species : Rat  
Sex : Male/female  
Strain : Sprague-Dawley  
Route of admin. : gavage  
Exposure period : 13 weeks  
Frequency of treatm. : Daily  
Post exposure period : 4 weeks  
Doses : 125, 350, 1000 mg/kg/day  
Control group : Yes  
NOAEL : 350 mg/kg bw  
NOEL : 125 mg/kg bw  
Method :  
Year : 1993  
GLP : Yes  
Test substance : Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4)  
Purity: >97% w/w

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- |               |   |
|---------------|---|
| <b>Method</b> | : Groups of 10 rats per sex per group were given doses of 0, 125, 350, or 1000 mg/kg/day by gavage, using a metal cannula for approximately 13 weeks. Dosing solutions were made daily and concentrations were analytically confirmed at weeks 1, 4, 8, and 13. The gavage vehicle was 1% carboxymethyl cellulose in water. Animals were housed in groups of 5 of the same sex and dose group per cage. The animal room was maintained at 19-25°C, 35-75% relative humidity, and a 12 hour light/12 hour dark lighting cycle. Rats were fed ad lib, but fasted -16 hours prior to blood sampling, during the collection of urine, and before necropsy. Water was also provided ad lib, but withheld during urine collection. All animals were observed twice daily for morbidity and mortality. Clinical observations were done daily, with full clinical evaluations done weekly. Body weights and food consumption were recorded weekly. Ophthalmoscopy was performed on all animals pretest and at week 13 in the control and high dose animals. Clinical pathology was performed on 10 animals/sex in control and high dose groups after week 4, 10 animals/sex in all groups after week 13, and in all recovery animals after week 17. Parameters included hematology (except on treatment-free period animals), blood clinical chemistry, and urinalysis. All animals were submitted to full necropsy. Organ weights were taken at necropsy. Histopathology was performed on all selected organs/tissues for all animals in the control and high dose groups, the liver, kidneys and lungs for all animals in all groups, and the heart from animals in groups 2 and 3 and in all recovery group animals. The hearts from all animals was examined after PTAH staining. |
| <b>Remark</b> | : Organs examined histologically also included the epididymides, mammary glands, ovaries, prostate, seminal vesicles, testes, uterus (horn + cervix). This is suggestive of no adverse effects on reproduction.   |
| <b>Result</b> | : There were no unscheduled deaths and no treatment related clinical signs. There were no treatment related differences in body weight gain and food consumption was unaffected by treatment. There were no treatment related eye lesions. None of the hematological parameters were considered to represent an adverse effect of treatment. None of the clinical chemistry parameters other than a reversible elevation in serum cholesterol in the high dose females and a reversible elevation of alanine and aspartate aminotransferase activities in all high dose animals were related to an effect of treatment. Urine parameters were unaffected other than being slightly more acidic in the high dose animals as compared to the controls. This was reversible after the 4 week treatment-free period. The minor differences in the weight of the major organs were considered of no toxicological significance in the absence of microscopic lesions. Macroscopic changes were considered to either be agonal or incidental in origin or unrelated to treatment. Treatment-related microscopic lesions were seen in the heart of high dose animals. The lesion was described as small foci of degenerated or necrotic fibers associated with minimal to moderate mononuclear cell  |

infiltration. This association suggested early or ongoing myocarditis. These lesions were not present in animals previously treated at the high dose level but allowed a 4 week period without treatment. There were no other treatment related microscopic lesions. In conclusion, the oral (gavage) administration of DLTDP to the rat for 13 weeks at a dose level of 1000 mg/kg/day was associated with a minor increase in serum cholesterol concentrations in females, increased serum ALAT and ASAT activities and decreased urinary pH in both sexes. Microscopic findings in the heart of these animals suggested an ongoing myocarditis. The heart was therefore identified as the target organ. All these changes were reversible after 4 weeks without treatment. At a dose level of 350 mg/kg/day there was no evidence for any treatment related microscopic change in the heart. Females at this dose exhibited a very small, but not statistically significant, increase in Hb concentrations. These individual values fell within the normal background range and are considered unlikely to be a direct toxic effect of the test material. Clinical chemistry results indicated calcium concentrations of the males were slightly elevated compared with controls. However, the differences were small, not statistically significant and generally well within the normal background range. No other differences to indicate an adverse effect of the test article were noted. This dose level is therefore considered to be the no observed adverse effect level for DLTDP in the rat. There were no changes considered to represent an effect of the test article at 125 mg/kg/day and therefore this dose level is considered to be the no observed effect level for DLTDP in the rat.

**Source**

:  
: 13 Week Oral (gavage) Toxicity Study in the Rat followed by a 4 Week Treatment-free Period. Ciba-Geigy Ltd. Base1 Switzerland. December 14, 1993.

**Reliability**

: This study is assigned a reliability code of 1b according to the criteria established by Klimisch et al. (1997). It was conducted under GLP guidelines but uses a non-specified protocol method that generally meets scientific standards, is well documented and is acceptable for assessment.

03.01.2004

(6)

**5.5 GENETIC TOXICITY 'IN VITRO'**

**Type** : Ames Test  
**System of testing** : 33.3, 100, 333, 1000, 2500, 3333, 5000, 6667 and 10,000 ug/plate and 3.3 and 10ug/plate for strain TA100.  
**Concentration** :  
**Cytotoxic conc.** : No toxicity was observed at 10,000 ug/plate with and without metabolic activation.  
**Metabolic activation** : With and without  
**Result** : Negative  
**Method** : Other: essentially follows OECD 471  
**Year** : 1979  
**GLP** : No

## 5. Toxicity

Id 4131-74-2

Date 08.05.2003

- 
- Test Substance** : Dilauryl thiodipropionate
- Method** : Tested with and without metabolic activation using Salmonella typhimurium strains TAI 535, TAI 537, TAI 538, TA98 and TAI 00 and Escherichia coli strain WP2. Liver S-9 fraction from Aroclor 1254 pretreated male Sprague-Dawley rats with NADPH generating system was used for metabolic activation. The experiment was repeated approximately 6 weeks later.
- Result** : Sodium azide was used as the positive control without metabolic activation while 2-anthramine was used as the positive control with metabolic activation. A precipitate was observed at the two highest doses tested. These plates were hand-counted. There was no evidence that it was mutagenic in the assays performed.
- Source** : SRI International (1979). Microbial mutagenesis testing of substances; compound report: F76-049, dilauryl thiodipropionate. NTIS report PB89169031.
- Reliability** : criteria established by Klimisch et al. (1997). It was not conducted under GLP guidelines but uses methods that generally meet scientific standards, is well documented and is acceptable for assessment.

03.01.2004

(6)

### 5.6 GENETIC TOXICITY 'IN VIVO'

- Type** : Dominant lethal assay
- Species** : Rat
- Sex** :
- Strain** : No data
- Route of admin.** : Gavage
- Exposure period** : An acute study and subacute study (dosed once/day for 5 days)
- Doses** : 50, 500 or 5000 mg/Kg
- Result** : Negative
- Method** : Other; essentially follows OECD 478
- Year** : 1973
- GLP** : No
- Test Substance** : Other; dilauryl thiodipropionic acid

## 5. Toxicity

Id 4131-74-2

Date 08.05.2003

- 
- Method** : Male and female rats from a closed colony were used. Animals were 10-12 weeks old at the time of use. Ten male rats were assigned to each of 5 groups; 3 dose levels of dilauryl thiodipropionic acid, 50, 500 or 5000 mg/kg, a positive control, triethylene melamine, and a negative control group. The positive control was administered intraperitoneally at a dose level of 0.3 mg/kg. Administration of the test compound was orally by intubation in both the acute study and in the subacute study (dosed once/day for 5 days). Following treatment, the males were sequentially mated to 2 females/week for 8 weeks (7 weeks in the subacute study). Two virgin female rats were housed with a male for 5 days (Monday through Friday). These two females were removed and housed in a cage until sacrificed. The males were left alone for two days and two new females were housed with a male for the next 5 days (Monday through Friday). Females were killed using carbon dioxide at 14 days after separation from the male and at necropsy the uterus was examined for early deaths, late fetal deaths and total implantations.
- Result** : There was no clear pattern of either increases or decreases between the control and test groups in any of the parameters studied. Thus, dilauryl thiodipropionic acid was considered to be non-mutagenic in rats in the dominant lethal assay when using the dosages employed in this study.
- Source** : Litton Bionetics, Inc (1973) Mutagenic evaluation of compound FDA 71-40, dilauryl thiodipropionic acid. NTIS PE3245452.
- Reliability** : This study is assigned a reliability code of 1b according to the criteria established by Klimisch et al. (1997). It was not conducted under GLP guidelines but uses methods that generally meet scientific standards, is well documented and is acceptable for assessment.

03.01.2004

(6)

### 5.7 GENETIC TOXICITY 'IN VIVO'

- Type** : Mouse Micronucleus  
**Species** : Rat  
**Sex** : Male  
**Strain** : No data  
**Route of admin.** : gavage  
**Exposure period** :  
**Doses** :  
**Result** : Negative  
**Method** : Other; essentially follows OECD 474 in vivo bone marrow mouse micronucleus test.  
**Year** : 1973  
**GLP** : No  
**Test Substance** : Other; dilauryl thiodipropionic acid

## 5. Toxicity

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- Method** : In the acute phase, groups of 5 male albino rats were sacrificed 6, 24 or 48 hours after dosing by oral gavage with 50, 500 or 5000 mg/kg dilauryl thiodipropionic acid. The negative control group of 9 rats received saline. The positive control group of 5 male rats melamine and was sacrificed hours prior to each sacrifice, colcemid intraperitoneally. received 0.3 mg/kg triethylene 48 hours after dosing. Two each animal received 4 mg/kg of Animals were sacrificed with carbon dioxide. The epiphysis of one femur was removed and the marrow aspirated into 5 ml of Hanks' balanced salt solution. The specimens were centrifuges at 1500 rpm for 5 minutes, decanted and 2 ml of hypotonic 0.5% KCl solution was aged with gentle agitation to resuspend the cells. The specimens were then placed in a 37C water bath for 20 minutes in order to swell the cells. Following centrifugation for 5 minutes at 1500 ppm, the supernatant was decanted and 2 ml of fixative (3:1 absolute methanol:glacial acetic acid) was added. The cells were resuspended in the fixative with gentile agitation, capped and maintained at 4C for 30 minutes. The specimens were again centrifuged, decanted, 2 ml of prepared fixative was added, and the cells were resuspended and maintained at 4C overnight. Cells were placed on a slide and stained with a 5% Giemsa solution for 20 minutes, rinsed in acetone, 1:1 acetone:xylene, and placed in fresh xylene for 30 minutes. Fifty metaphase spreads were scored per animal. Mitotic indices were obtained by counting at least 500 cells and the ratio of the number of cells in mitosis/the number of cells observed was expressed as the mitotic index.
- Result** : The compound produced no detectable significant aberration of the bone marrow metaphase chromosomes of rats when administered orally at the dosage levels employed in this study following acute or short term exposure. Mitotic indices were normal.
- Source** : Litton Bionetics, Inc (I 973) Mutagenic evaluation of compound FDA 71-40, dilauryl thiodipropionic acid. NTIS PB245452.
- Reliability** : This study is assigned a reliability code of 1b according to the criteria established by Klimisch ef al. (1997). It was not conducted under GLP guidelines but uses methods that generally meet scientific standards, is well documented and is acceptable for assessment.

03.01.2004

(6)

### 5.8.1 TOXICITY TO FERTILITY

- Type** : other  
**Species** : rat  
**Sex** : male/female  
**Strain** : Sprague-Dawley  
**Route of admin.** : gavage  
**Exposure period** : 13 weeks + 4 weeks post exposure

## 5. Toxicity

Id 4131-74-2  
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Frequency of treatm. : daily  
Premating exposure period  
    Male :  
    Female :  
Duration of test :  
No. of generation :  
studies :  
Doses : 125, 350, 1000 mg/kg/day  
Control group :  
Method :  
Year : 1993  
GLP : yes  
Test substance : Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4)  
Purity: >97% w/w

Method : Test subjects:

Age at study initiation: 6 weeks, males 162-193g, females 142-180g.

No. of animals/sex/dose: 10 rats/sex/group

Study Design:

Vehicle: 1% carboxymethyl cellulose in water.

Clinical observations:

All animals were observed twice daily for morbidity and mortality. Clinical observations were done daily, with full clinical evaluations done weekly. Body weights and food consumption were recorded weekly. Ophthalmoscopy was performed on all animals pretest and at week 13 in the control and high dose animals. Clinical pathology was performed on 10 animals/sex in control and high dose groups after week 4, 10 animals/sex in all groups after week 13, and in all recovery animals after week 17. Parameters included hematology (except on treatment-free period animals), blood clinical chemistry and urinalysis.

Organs examined at necropsy: All animals were submitted to full necropsy. Organ weights were taken at necropsy. Histopathology was performed on all selected organs/tissues for all animals in the control and high dose groups, the liver, kidneys and lungs for all animals in all groups, and the heart from animals in groups 2 and 3 and in all recovery group animals. The hearts from all animals were examined after PTAH staining. Organs examined histologically also included the epidymides, mammary glands, ovaries, prostate, seminal vesicles, testes, uterus (horn + cervix).

Result : NOAEL = 350 mg/kg/day

NOEL = 125 mg/kg/day

Body weight: No treatment related differences in body weight gain.

Food/water consumption: Unaffected by treatment.

Mortality: No unscheduled deaths.

## 5. Toxicity

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Clinical signs: No treatment related clinical signs

Ophthalmology: No treatment related eye lesions.

Hematology: None of the hematologic parameters were considered to represent an adverse effect of treatment.

Urine: Urine parameters were unaffected other than being slightly more acidic in the high dose animals as compared to the controls. This was reversible after the 4 week treatment-free period.

Clinical chemistry: None of the clinical chemistry parameters other than a reversible elevation in serum cholesterol in the high dose females and a reversible elevation of alanine and aspartate aminotransferase activities in all high dose animals were related to an effect of treatment.

Gross pathology: Macroscopic changes were considered to either be agonal or incidental in origin or unrelated to treatment. Treatment related microscopic lesions were seen in the heart of high dose animals. The lesion was described as small foci of degenerated or necrotic fibers associated with minimal to moderate mononuclear cell infiltration. This association suggested early or ongoing myocarditis. These lesions were not present in animals previously treated at the high dose level but allowed a 4 week period without treatment. There were no other treatment related microscopic lesions.

Organ weight changes: Minor differences in the weight of the major organs were considered of no toxicological significance in the absence of microscopic lesion.

### Conclusion

: This study included specific evaluation of the reproductive organs of the test animals. No adverse effects on these organs were seen at the dose levels used in this study. This is suggestive of no adverse effects on reproduction.

Reliability  
07.05.2003

: (2) valid with restrictions

(1)

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	days 6-15 of gestation
Frequency of treatm.	:	
Duration of test	:	
Doses	:	16, 74, 350 or 1600 mg/kg in corn oil
Control group	:	yes
NOAEL maternal tox.	:	1600 mg/kg bw
NOAEL teratogen.	:	1600 mg/kg bw
Method	:	other: essentially follows OECD 414
Year	:	1972
GLP	:	no

## 5. Toxicity

Id 4131-74-2

Date 08.05.2003

- 
- Test substance** : Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4)  
Purity: not stated
- Method** : A positive control group received 250 mg/kg aspirin. Frequency of treatment for positive control group not stated. The number of pregnant rats at the end of the study ranged from 19-21/dose level. Feed and water were available ad libitum. The rats were observed daily for general appearance and behaviour, with emphasis on feed consumption and weight. Weights were obtained on days 0, 6, 11, 15 and 20 of gestation. On day 20 of gestation caesarian sections were performed and the numbers of implantation and resorption sites as well as the numbers of live and dead fetuses were recorded. The urogenital tract of each dam was examined for any abnormality, all fetuses were examined for any gross external abnormalities, and all live pups were weighed. Visceral examinations were performed on one-third of the fetuses of each litter, and the remaining two-thirds were examined for skeletal defects.
- Result** : No adverse effects with respect to number of implantations and maternal or fetal death were noted after oral administration to rats of up to 1600 mg/kg dilauryl thiodipropiionic acid on days 6-15 of gestation. There were no significant differences in numbers of abnormalities of the soft or skeletal tissues between the treated and sham control fetuses.
- Reliability** : (2) valid with restrictions (4)  
07.05.2003
- Species** : mouse  
**Sex** : female  
**Strain** : CD-1  
**Route of admin.** : gavage  
**Exposure period** : days 6-15 of gestation  
**Frequency of treatm.** : daily  
**Duration of test** :  
**Doses** : 16, 74, 350 and 1600 mg/kg in corn oil  
**Control group** : yes  
**NOAEL maternal tox.** : 1600 mg/kg bw  
**NOAEL teratogen.** : 1600 mg/kg bw  
**Method** : other: essentially follows OECD 414  
**Year** : 1972  
**GLP** : no
- Test substance** : Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4)  
Purity: not stated
- Method** : A positive control group received 150 mg/kg aspirin. Frequency of treatment for the positive control not stated. The number of pregnant mice at the end of the study ranged from 20-22/dose level. Feed and water were available ad libitum. The mice were observed daily for general appearance and behaviour, with emphasis on feed consumption and weight. Weights were obtained on days 0, 6, 11, 15 and 17 of gestation. On day 17 of gestation, caesarian sections were performed and the numbers of implantation and resorption sites, as well as the numbers of live and dead fetuses, were recorded. The urogenital tract of each dam was examined for any abnormality, all fetuses were examined for any gross external abnormalities, and all live pups were weighed. Visceral examinations were performed on one-third of the fetuses of each litter, and

## 5. Toxicity

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<b>Result</b>	: the remaining two-thirds were examined for skeletal defects. : No adverse effects were found with respect to implantations and maternal and fetal survival after oral administration to mice of up to 1600 mg/kg test material on days 6-15 of gestation. The number of abnormalities seen in the soft or skeletal tissues of the treated fetuses was comparable to that seen in the sham control fetuses.
<b>Reliability</b> 07.05.2003	: (2) valid with restrictions (4)
<b>Species</b>	: rabbit
<b>Sex</b>	: female
<b>Strain</b>	: Dutch
<b>Route of admin.</b>	: gavage
<b>Exposure period</b>	: days 6-18 of gestation
<b>Frequency of treatm.</b>	: daily
<b>Duration of test</b>	:
<b>Doses</b>	: 2.5, 10, 45, 216, 1000 mg/kg in corn oil
<b>Control group</b>	: yes
<b>NOAEL maternal tox.</b>	: 1000 mg/kg bw
<b>NOAEL teratogen.</b>	: 1000 mg/kg bw
<b>Method</b>	: other: essentially follows OECD 414
<b>Year</b>	: 1973
<b>GLP</b>	: no
<b>Test substance</b>	: Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4) Purity: not stated
<b>Method</b>	: Groups of 15-29 artificially inseminated females/dose level resulted in 8-13 pregnant rabbits/dose level. On day 29, all does were subjected to caesarian section. The numbers of corpora lutea, implantation sites, resorption sites, and live and dead fetuses were recorded. The body weights of the live pups were also recorded. The urogenital tract of each animal was examined in detail for normality. All fetuses underwent a detailed gross examination for the presence of external congenital abnormalities. The live fetuses of each litter were then placed in an incubator for 24 hours for the evaluation of neonatal survival. All surviving pups were sacrificed, and all pups examined for visceral abnormalities by dissection. All fetuses were then cleared in potassium hydroxide, stained with alizarin red S dye and examined for skeletal defects.
<b>Result</b>	: Eight to thirteen pregnant dams survived to term. There was no clearly discernible effect on nidation or on maternal or fetal survival at doses as high as 1000 mg/kg. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring spontaneously in the control.
<b>Reliability</b> 07.05.2003	: (2) valid with restrictions (3)
<b>Species</b>	: hamster
<b>Sex</b>	: female
<b>Strain</b>	: other: Golden
<b>Route of admin.</b>	: gavage
<b>Exposure period</b>	: days 6-10 of gestation
<b>Frequency of treatm.</b>	: daily
<b>Duration of test</b>	:
<b>Doses</b>	: 16, 74, 350 or 1600 mg/kg in corn oil

## 5. Toxicity

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<b>Control group</b>	:	yes
<b>NOAEL maternal tox.</b>	:	1600 mg/kg bw
<b>NOAEL teratogen.</b>	:	1600 mg/kg bw
<b>Method</b>	:	other: essentially follows OECD 414
<b>Year</b>	:	1972
<b>GLP</b>	:	no
<b>Test substance</b>	:	Chemical name: 3,3'-thiodipropionic acid, didodecyl ester (CAS No. 123-28-4) Purity: not stated
<b>Method</b>	:	The number of hamsters at the end of the study ranged from 20-23/dose level. Feed and water were available ad libitum. The hamsters were observed daily for general appearance and behaviour, with emphasis on feed consumption and weight. Weights were obtained on days 0, 8, 10 and 14 of gestation. On day 14 of gestation caesarian sections were performed and the numbers of implantation and resorption sites as well as the numbers of live and dead fetuses were recorded. The urogenital tract of each dam was examined for any abnormality, all fetuses were examined for any gross external abnormalities, and all live pups were weighed. Visceral examinations were performed on one-third of the fetuses of each litter, and the remaining two-thirds were examined for skeletal defects.
<b>Result</b>	:	The numbers of implantations and maternal and fetal survival were not adversely affected by oral administration to hamsters of up to 1600 mg/kg test material on days 6-10 of gestation. No significant differences in the number of soft or skeletal tissue abnormalities were found between treated and sham control fetuses.
<b>Reliability</b> 07.05.2003	:	(2) valid with restrictions

(4)

## 9. References

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