

Safety Data Sheet**THL-Hydroxy- β -lactone**

according to Regulation (EU) nr. 1907/2006

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**Product name THL-Hydroxy- β -lactone

Product code 04 2113 8

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use - intermediate product in the synthesis of tetrahydrolipstatin

1.3. Details of the supplier of the safety data sheet

Company information

Enquiries:
F. Hoffmann-La Roche AG
Postfach
CH-4070 Basel
Switzerland

Local representation:

Phone +41-61/688 54 80
Fax +41-61/681 72 76
E-Mail info.sds@roche.com**1.4. Emergency telephone number**

Emergency telephone number Phone +41-61/688 54 80

THL-Hydroxy- β -lactone

SECTION 2: Hazards identification

2.1. / 2.2. Classification of the substance or mixture / Label elements

GHS Classification

Environmental Hazards:

4.1 Hazardous to the aquatic environment (Category 1)

H400 Very toxic to aquatic life.

4.1 Hazardous to the aquatic environment (Category 1)

H410 Very toxic to aquatic life with long lasting effects.

Signalword: Warning

Label:



Precautionary statements:

- P273 Avoid release to the environment.
- P312 Call a POISON CENTER or doctor/physician if you feel unwell.
- P501 Dispose of contents/container to waste disposal as hazardous waste

2.3. Other hazards

Note

- may form explosible dust-air mixture if dispersed

SECTION 3: Composition/information on ingredients

Chemical name

- (3S,4S)-3-Hexyl-4-[(R)-2-hydroxytridecyl]-2-oxetanone

Synonyms

- Hydroxy- β -lactone
- THL-HBL
- HBL

CAS number

104872-06-2

ELINCS number

418 650 2

UN number

3077

Roche number

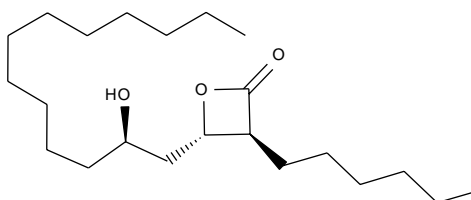
Ro0193052-000

Empirical formula

C₂₂H₄₂O₃

Molecular mass

354.58 g/mol



SECTION 4: First aid measures

4.1. Description of first aid measures

- | | |
|--------------|---|
| Eye contact | <ul style="list-style-type: none">- rinse immediately with tap water for at least 20 minutes - open eyelids forcibly- consult a physician |
| Skin contact | <ul style="list-style-type: none">- remove immediately contaminated clothes, wash affected skin with water and soap - do not use any solvents |
| Inhalation | <ul style="list-style-type: none">- remove the casualty to fresh air and keep him/her calm- in the event of symptoms get medical treatment |

4.2. Most important symptoms and effects, both acute and delayed

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|------|--|
| Note | <ul style="list-style-type: none">- no information available |
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4.3. Indication of any immediate medical attention and special treatment needed

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|-------------------|---|
| Note to physician | <ul style="list-style-type: none">- treat symptomatically |
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SECTION 5: Firefighting measures

5.1. Extinguishing media

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|--------------------------------|--|
| Suitable extinguishing media | <ul style="list-style-type: none">- foam, powder, carbon dioxide |
| Unsuitable extinguishing media | <ul style="list-style-type: none">- use water spray for cooling purposes only (fat explosion hazard) |

5.2. Special hazards arising from the substance or mixture

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|------------------|---|
| Specific hazards | <ul style="list-style-type: none">- consider dust explosion hazard- substance is hazardous for water: contain fire-fighting wastewater |
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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

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|----------------------|---|
| Personal precautions | <ul style="list-style-type: none">- no special precautions required |
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6.2. Environmental precautions

- | | |
|--------------------------|---|
| Environmental protection | <ul style="list-style-type: none">- do not allow to enter drains or waterways- if the substance reaches waters or the sewer system, inform the competent authority |
|--------------------------|---|

6.3. Methods and material for containment and cleaning up

Methods for cleaning up	- collect solids (avoid dust formation) and hand over to waste removal
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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Technical measures	<ul style="list-style-type: none">- processing in closed systems, if possible superposed by inert gas (e.g. nitrogen)- local exhaust ventilation necessary- take precautionary measures against electrostatic charging- avoid dust formation; very high dust explosion hazard
Suitable materials	- stainless steel, aluminium, glass, enamel, polyethylene

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions	<ul style="list-style-type: none">- room temperature- protected from humidity
Validity	- 24 months, 15 to 25 °C
Packaging materials	- tightly closing; material: cardboard, steel, plywood (lined with polyethylene bag)

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Note	- no information available
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8.2. Exposure controls

Respiratory protection	- in case of open handling or accidental release: particle mask or respirator with independent air supply
Hand protection	- protective gloves (neoprene, nitrile or butyl rubber)
Eye protection	- safety glasses
Analytics	- sampling on glass fibre filter and gravimetric or chemical determination

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Form	fine powder
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THL-Hydroxy- β -lactone

Odour	odourless
Density	0.94 g/cm ³ (22 °C; OECD No. 109)
Solubility	1'000 mg/l, hexane 20'000 mg/l, methanol 100'000 mg/l, tetrahydrofuran < 0.02 mg/l, water (20 °C, A.6. EG method)
Partition coefficient	log P _{ow} 10.4 (24 °C) (HPLC Method, OECD No. 117)
Melting temperature	61.4 to 63.3 °C (OECD No. 102)
Boiling temperature	> 200 °C with decomposition
Vapour pressure	< 10 Pa (60 °C) (OECD No. 104)
Ignition point (liquid)	250 °C

9.2. Other information

Bulk density	~ 0.35 g/cm ³
Particle size	79 % < 5 μ m 92 % < 100 μ m (OECD No. 110)

SECTION 10: Stability and reactivity

10.1. Reactivity

Note	- no information available
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10.2. Chemical stability

Note	- no information available
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10.3. Possibility of hazardous reactions

Note	- no information available
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10.4. Conditions to avoid

Conditions to avoid	- warming - humidity
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10.5. Incompatible materials

Materials to avoid	- oxidizing agents, acids, bases
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10.6. Hazardous decomposition products

Note - not explosible when exposed to thermal or mechanical (shock, friction) stress

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity	- LD ₅₀ > 2'000 mg/kg (oral, rat)
	- LD ₅₀ > 2'000 mg/kg (dermal)
Subacute toxicity	- NOAEL 1'000 mg/kg/d (oral, rat, 28 days)
Local effects	- skin: non-irritant (rabbit)
	- eye: non-irritant (rabbit)
Sensitization	- not sensitizing (guinea pig)
Mutagenicity	- not mutagenic (various in vitro test systems)
Carcinogenicity	- no information available
Reproductive toxicity	- no information available
STOT-single exposure	- no information available
STOT-repeated exposure	- no information available
Aspiration hazard	- no information available
Note	- no toxic effects have been observed during occupational handling

SECTION 12: Ecological information

12.1. Toxicity

Ecotoxicity	- highly toxic for algae (<i>Scenedesmus</i> (=Desmodesmus) subspicatus) NOEC (72 h) 0.063 mg/l (nominal concentration) EbC ₅₀ (72 h) 0.40 mg/l (nominal concentration) (OECD No. 201)
	- highly toxic for planktonic crustaceans (<i>Daphnia magna</i>) NOEC (48 h) 0.01 mg/l (nominal concentration) EC ₅₀ (48 h) 0.058 mg/l (nominal concentration) (OECD No. 202)
	- barely toxic for fish (nominal concentration = 100 mg/l) (rainbow trout) NOEC (96 h) 100 mg/l LC ₅₀ (96 h) > 100 mg/l (OECD No. 203)

THL-Hydroxy- β -lactone

- barely toxic for microorganisms (nominal concentration = 100 mg/l) (activated sludge)
NOEC 100 mg/l
(Activated Sludge Respir. Inhib. Test, OECD No. 209)

12.2. Persistence and degradability

- Ready biodegradability
- not readily biodegradable
18.4 %, 28 d
(Manometric Respirometry Test, OECD No. 301 F)

12.3. Bioaccumulative potential

- Note
- no information available

12.4. Mobility in soil

- Note
- no information available

12.5. Results of PBT and vPvB assessment

- Note
- no information available

12.6. Other adverse effects

- Air pollution
- observe local/national regulations

SECTION 13: Disposal considerations

13.1. Waste treatment methods

- Waste from residues
- incinerate in qualified installation with flue gas scrubbing
 - observe local/national regulations regarding waste disposal
- Contaminated packaging
- incinerate contaminated packaging material in qualified installation with flue gas scrubbing

SECTION 14: Transport information

IATA	Class	UN/ID	PG		PI	Label	Mark
	9	3077	III		956/956	9	EHS
IMDG	Class	UN	PG	EmS	PI	Label	Mark
	9	3077	III	F-A S-F	P002/IBC08	9	marine pollutant

THL-Hydroxy- β -lactone

RID/ADR	Class	UN	PG	Haz.no	PI	Label	Mark	Classif. code
	9	3077	III	90	P002/IBC08	9	EHS	M7

Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

Technical name (3S,4S)-3-Hexyl-4-[(R)-2-hydroxytridecyl]-2-oxetanone

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

Water hazard class (Germany) 2: hazardous for water (own classification according to directive VwVwS of 17.05.1999)

SECTION 16: Other information

Safety-lab number

- BS-5354
- BS-5727
- BS-5728

Edition documentation

- changes from previous version in sections 2

The information in this safety data sheet is based on current scientific knowledge. It should not be taken as expressing or implying any warranty concerning product characteristics.