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Safety Data Sheet

according to UK REACH Regulation

3-O-Trityl-6-O-desmethyl-buprenorphine

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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

3-O-Trityl-6-O-desmethyl-buprenorphine

Further trade names

6,14-Ethenomorphinan-7-methanol, 17-(cyclporopyl-methyl)-alpha-(1,1-dimethylethyl) -4,5-epoxy-18,19-dihydro-6-hydroxy-alpha-methyl-3-(triphenylmethoxy)-, (5alpha, 7alpha(S))

Synonymes: TDBPN

CAS No: 157891-93-5

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

Use of the substance/mixture

Precursor for 6-O-[11C]-buprenorphine

1.3. Details of the supplier of the safety data sheet

Company name: ABX advanced biochemical compounds

Biomedizinische Forschungsreagenzien GmbH

Street: Heinrich-Gläser-Straße 10-14

Place: 01454 Radeberg
Telephone: +49 3528 4041 60

e-mail: info@abx.de

Contact person: Dr. Christoph Meyer Telephone: +49 3528 4041 8732

e-mail: meyer@abx.de Internet: http://www.abx.de

1.4. Emergency telephone +49 3528 4041 60

number:

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

GB CLP Regulation

Acute Tox. 4; H312 Acute Tox. 4; H302 Skin Irrit. 2; H315 Eye Irrit. 2; H319

Full text of hazard statements: see SECTION 16.

2.2. Label elements

GB CLP Regulation

Hazard components for labelling

3-O-Trityl-6-O-desmethyl-buprenorphine

Signal word: Warning

Pictograms:



Hazard statements

H302+H312 Harmful if swallowed or in contact with skin.

H315 Causes skin irritation. H319 Causes serious eye irritation.

according to UK REACH Regulation

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H335 May cause respiratory irritation.

Precautionary statements

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing

protection.

2.3. Other hazards

Warning - substance not yet tested completely. Bridging principle ' Substantially similar mixtures.'

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical characterization

6,14-Ethenomorphinan-7-methanol, 17-(cyclporopyl-methyl)-alpha-(1,1-dimethylethyl) -4,5-epoxy-18,19-dihydro-6-hydroxy-alpha-methyl-3-(triphenylmethoxy)-, (5alpha, 7alpha(S))

Sum formula: C47H53NO4 Molecular weight: 695.93

Hazardous components

CAS No	Chemical name				
	EC No	Index No	REACH No		
	Classification (GB CLP Regulation)				
157891-93-5	3-O-Trityl-6-O-desmethyl-buprenorphine				
	Acute Tox. 4, Acute Tox. 4, Skin Irrit. 2, Eye Irrit. 2; H312 H302 H315 H319				

Full text of H and EUH statements: see section 16.

Specific Conc. Limits. M-factors and ATE

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CAS No	EC No	Chemical name	Quantity	
	Specific Conc. Limits, M-factors and ATE			
157891-93-5		3-O-Trityl-6-O-desmethyl-buprenorphine	95 - < 100 %	
	dermal: ATE =	1100 mg/kg; oral: ATE = 500 mg/kg		

SECTION 4: First aid measures

4.1. Description of first aid measures

After inhalation

Provide fresh air.

After contact with skin

After contact with skin, wash immediately with: Water. Change contaminated clothing.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

If swallowed, immediately drink: Water. Call a physician immediately.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings. Suitable extinguishing media: Foam. Extinguishing powder. Carbon dioxide (CO2). Atomized water.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

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Additional information

Contaminated fire-fighting water must be collected separately. Do not allow to enter into surface water or

SECTION 6: Accidental release measures

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

Other information

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Do not breathe dust. Conditions to avoid: skin contact. Eye contact. Wear personal protection equipment.

When using do not eat, drink, smoke, sniff.

Advice on general occupational hygiene

Change contaminated clothing. Wash hands before breaks and after work. When using do not eat or drink.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container dry. Keep container tightly closed.

Further information on storage conditions

Recommended storage temperature:

of °C: -25 up to °C: -15 Protect against: Light. Store under (Gas): argon.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Additional advice on limit values

To date, no national critical limit values exist.

8.2. Exposure controls

Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state: solid

Colour: colourless , light yellow

Changes in the physical state Solubility in other solvents

Chloroform , Dichloromethane: Ethanol

SECTION 10: Stability and reactivity

10.4. Conditions to avoid

Light.

according to UK REACH Regulation

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10.6. Hazardous decomposition products

Carbon dioxide. Carbon monoxide. Nitrogen oxides (NOx).

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in GB CLP Regulation

Acute toxicity

CAS No	Chemical name						
	Exposure route	Dose	Species	Source	Method		
157891-93-5	3-O-Trityl-6-O-desmethyl-buprenorphine						
	oral	ATE 500 mg/kg					
	dermal	ATE 1100 mg/kg					

Further information

Toxicological data are not available.

SECTION 12: Ecological information

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of UK REACH.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Do not allow to enter into surface water or drains. Dispose of waste according to applicable legislation.

List of Wastes Code - residues/unused products

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and

discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

List of Wastes Code - used product

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and

discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances: hazardous waste

List of Wastes Code - contaminated packaging

150110 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND

PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); packaging containing residues of or contaminated by hazardous substances; hazardous waste

Contaminated packaging

Non-contaminated packages may be recycled.

SECTION 14: Transport information

Other applicable information

Not a hazardous material with respect to these transportation regulations.

according to UK REACH Regulation

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SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 75

National regulatory information

Water hazard class (D): 3 - highly hazardous to water

SECTION 16: Other information

Relevant H and EUH statements (number and full text)

H302 Harmful if swallowed.

H302+H312 Harmful if swallowed or in contact with skin.

H312 Harmful in contact with skin. H315 Causes skin irritation.

H319 Causes serious eye irritation.
H335 May cause respiratory irritation.