

# **Safety Data Sheet**

acc. to OSHA HCS

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## **1** Identification

- · Product identifier
- · Trade name: (±)-cis-3-methyl Norfentanyl
- · Synonym 3-Methylfentanyl metabolite
- · Other means of identification

#### · Article number: 22617

- · Application of the substance / the mixture This product is for research use - Not for human or veterinary diagnostic or therapeutic use.
- · Details of the supplier of the safety data sheet
- Manufacturer/Supplier: Cayman Chemical Co. 1180 E. Ellsworth Rd. Ann Arbor, MI 48108 USA
- · Information department: Product safety department Emergency telephone number: During normal opening times: +1 (734) 971-3335
- US/CANADA: 800-424-9300 Outside US/CANADA: 703-741-5970

# 2 Hazard(s) identification

· Classification of the substance or mixture			
GHS02 Flame			
Flammable liquids 2	H225 Highly flammable liquid and vapor.		
GHS07 Acute toxicity - oral 4	H302 Harmful if swallowed.		
•	H312 Harmful in contact with skin.		
Acute toxicity - inhalation 4			
Eye irritation 2A	H319 Causes serious eye irritation.		
<ul> <li>Label elements</li> <li>GHS label elements</li> <li>The product is classified an</li> </ul>	id labeled according to the Globally Harmonized System (GHS). (Contd. on page 2)		

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Hazard pictog	rams (Contd. from page
Jul I	
<u>**</u>	
GHS02 GHS	07
Signal word Da	anger
Hazard-determ Acetonitrile	nining components of labeling:
(±)-cis-3-methy	l Norfontanyl
Hazard statem	
H225	Highly flammable liquid and vapor.
	332 Harmful if swallowed, in contact with skin or if inhaled.
H319	Causes serious eye irritation.
Precautionary	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition source
	No smoking.
P233	Keep container tightly closed.
P240	Ground / bond container and receiving equipment.
P241	Use explosion-proof [electrical/ventilating/lighting] equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharge.
P261	Avoid breathing dust/fume/gas/mist/vapors/spray
P264	Wash thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearin protection.
P301+P312	If swallowed: Call a poison center/doctor if you feel unwell.
P303+P361+P3	353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin wi water [or shower].
P304+P340	If inhaled: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P3	338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses present and easy to do. Continue rinsing.
P321	Specific treatment (see on this label).
P330	Rinse mouth.
P362+P364	Take off contaminated clothing and wash it before reuse.
P337+P313	If eye irritation persists: Get medical advice/attention.
P370+P378	In case of fire: Use CO2, powder or water spray to extinguish.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/container in accordance with local/regional/national/internation
Information	regulations.
Classification	ertaining to particular dangers for man and environment:
NFPA ratings (	
in FA launys (	
He He	ealth = 2
	re = 3
<b>20</b> Re	eactivity = 0
▼ ∨	

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· HMIS-ratings (scale 0 - 4)

HEALTH 2	Health = 2
	Fire = 3
REACTIVITY 0	Reactivity = 0

#### · Other hazards

- · Results of PBT and vPvB assessment
- **PBT:** Not applicable.
- vPvB: Not applicable.
- Classification according to (d)(1)(ii) of § 1910.1200

The SDS issuer does not object to the classifications provided by importers or manufacturers of precursor products.

· Hazards not otherwise classified

There are no adverse physical or health effects known that are not covered by the hazard classes of the Hazard Communications Standard.

### **3 Composition/information on ingredients**

#### · Chemical characterization: Mixtures

• Description: Mixture of the substances listed below with nonhazardous additions.

#### · Dangerous components:

· J· · · · · ·		
CAS: 75-05-8	Acetonitrile	99.0%
RTECS: AL7700000		
CAS: 33794-42-2	(±)-cis-3-methyl Norfentanyl	1.0%

#### **4 First-aid measures**

#### Description of first aid measures

• General information:

Immediately remove any clothing soiled by the product.

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

• After inhalation:

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

- In case of unconsciousness place patient stably in side position for transportation.
- After skin contact: Immediately rinse with water.
- · After eye contact:

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

- After swallowing: Immediately call a doctor.
- Most important symptoms and effects, both acute and delayed No further relevant information available.
- Indication of any immediate medical attention and special treatment needed No further relevant information available.

### **5 Fire-fighting measures**

- · Extinguishing media
- Suitable extinguishing agents:

CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

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13 ppm

50 ppm

150 ppm

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(Contd. from page 3) • Special hazards arising from the substance or mixture No further relevant information available. • Advice for firefighters

• Protective equipment: Mouth respiratory protective device.

#### 6 Accidental release measures

- Personal precautions, protective equipment and emergency procedures Wear protective equipment. Keep unprotected persons away.
- Environmental precautions:
- Dilute with plenty of water.

Do not allow to enter sewers/ surface or ground water.

• Methods and material for containment and cleaning up:

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust). Dispose contaminated material as waste according to section 13. Ensure adequate ventilation.

Protective Action Criteria for Chemicals

· PAC-1:

75-05-8 Acetonitrile

· PAC-2:

75-05-8 Acetonitrile

· PAC-3:

75-05-8 Acetonitrile

· Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

### 7 Handling and storage

• **Precautions for safe handling** Ensure good ventilation/exhaustion at the workplace. Prevent formation of aerosols.

 Information about protection against explosions and fires: Keep ignition sources away - Do not smoke.
 Protect against electrostatic charges.

#### · Conditions for safe storage, including any incompatibilities

- · Storage: Store in accordance with information listed on the product insert.
- Requirements to be met by storerooms and receptacles: Store in a cool location.
- · Information about storage in one common storage facility: Not required.
- Further information about storage conditions: Keep receptacle tightly sealed. Store in cool, dry conditions in well sealed receptacles.
- · Specific end use(s) No further relevant information available.

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### 8 Exposure controls/personal protection

#### · Control parameters

· Components with limit values that require monitoring at the workplace:

The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.

At this time, the remaining constituent has no known exposure limits.

#### 75-05-8 Acetonitrile

PEL Long-term value: 70 mg/m<sup>3</sup>, 40 ppm

- REL Long-term value: 34 mg/m<sup>3</sup>, 20 ppm
- TLV Long-term value: 20 ppm
  - Skin, A4

· Additional information: The lists that were valid during the creation were used as basis.

#### • Exposure controls

- · Appropriate engineering controls No further data; see section 7.
- Personal protective equipment:
- General protective and hygienic measures:

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes. Avoid contact with the eyes and skin.

· Breathing equipment:

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

#### • Protection of hands:



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

#### · Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

#### · Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

#### · Eye protection:



Tightly sealed goggles

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Information on basic physical and chemic	al properties
General Information	
Physical state	Liquid
Color:	According to product specification
Odor:	Aromatic
Structural Formula	C15H22N2O
Molecular Weight	246.4 g/mol
Storage Buffer	240.4 g/mol
Odor threshold:	Not determined.
Formulation	A solution in acetonitrile
Melting point/Melting range:	-46 °C (-50.8 °F)
Boiling point/Boiling range:	81 °C (177.8 °F)
Flammability:	Highly flammable.
Explosion limits:	4 4 \/ol 9/
Lower:	4.4 Vol %
Upper:	16 Vol %
Flash point:	2 °C (35.6 °F)
Auto igniting:	525 °C (977 °F)
Decomposition temperature:	Not determined.
pH-value:	Not determined.
Viscosity:	
Kinematic:	Not determined.
SOLUBILITY	DMF: 30 mg/mL; DMSO: 20 mg/mL; Ethanol: 30 mg
	mL; PBS (pH 7.2): 10 mg/mL
Dynamic at 20 °C (68 °F):	0.35 mPas
Solubility in / Miscibility with	
Water at 25 °C (77 °F):	1000 g/l
Partition coefficient (n-octanol/water):	Not determined.
Vapor pressure at 20 °C (68 °F):	98.64 hPa (74 mm Hg)
Vapor pressure at 50 °C (122 °F):	330 hPa (247.5 mm Hg)
Density at 20 °C (68 °F):	0.79 g/cm <sup>3</sup> (6.59255 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Particle characteristics	Not applicable.
	······································
Other information	
Appearance:	
Form:	Liquid
Important information on protection of hea	alth
and environment, and on safety.	
Ignition temperature:	Product is not selfigniting.
Danger of explosion:	Product is not explosive. However, formation o
	explosive air/vapor mixtures are possible.
Solvent content:	
VOC content:	0.00 %
	0.0 g/l / 0.00 lb/gal
Solids content:	1.0 %
Change in condition	

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# **10 Stability and reactivity**

- · Reactivity No further relevant information available.
- · Chemical stability
- Thermal decomposition / conditions to be avoided:

No decomposition if used according to specifications.

- Possibility of hazardous reactions No dangerous reactions known.
- · Conditions to avoid No further relevant information available.
- · Incompatible materials: No further relevant information available.
- · Hazardous decomposition products: No dangerous decomposition products known.

· Informatio		cological effects
	•	at are relevant for classification:
ATE (Acu	te Toxicity	y Estimate)
Oral	LD50	616 mg/kg
Dermal	LD50	1,495 mg/kg
Inhalative	LC50/4 h	10.3 mg/l
75-05-8 A	cetonitrile	· · · · · · · · · · · · · · · · · · ·
Oral	LD50	617 mg/kg (mouse) (OECD Test Guideline 401)
Dermal	LD50	1,500 mg/kg (rabbit) (Expert Judgement) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Inhalative	LC50/4 h	6.022 mg/l (mouse) (OECD Test Guideline 403)
<ul> <li>Additiona</li> <li>The produce</li> <li>preparation</li> <li>Harmful</li> <li>Irritant</li> </ul>	e: Irritating tion: No se Il toxicolo uct shows ns:	
Carcinog		
-	-	Agency for Research on Cancer)
•		nts is listed.
· NTD /Nati	onal Toxi	cology Program)
111 F (11au		
None of th	le ingredie	
None of th	<u> </u>	ional Safety & Health Administration)

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#### · Alternative sources for toxicological information

No non-standard sources for toxicological information where used.

#### **12 Ecological information**

- · Toxicity
- · Aquatic toxicity: No further relevant information available.
- Persistence and degradability No further relevant information available.
- · **Bioaccumulative potential** No further relevant information available.
- · Mobility in soil No further relevant information available.
- · Results of PBT and vPvB assessment
- · **PBT:** Not applicable.
- · vPvB: Not applicable.
- Other adverse effects
- · Additional ecological information:
- · General notes:

Water hazard class 2 (Self-assessment): hazardous for water

- Do not allow product to reach ground water, water course or sewage system.
- Danger to drinking water if even small quantities leak into the ground.

### **13 Disposal considerations**

- · Waste treatment methods
- · Recommendation:

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

- · Uncleaned packagings:
- Recommendation: Disposal must be made according to official regulations.
- Recommended cleansing agent: Water, if necessary with cleansing agents.

UN-Number		
DOT, IMDG, IATA	UN1648	
UN proper shipping name		
DOT, IATA	Acetonitrile solution	
IMDG	ACETONITRILE solution	
Transport hazard class(es)		
DOT		
PLAMABLE LOUD		
3		

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· Label	3
· IMDG, IATA	
· Class · Label	3 Flammable liquids 3
· Packing group · DOT, IMDG, IATA	II
· Environmental hazards:	Not applicable.
<ul> <li>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</li> </ul>	Not applicable.
<ul> <li>Transport/Additional information:</li> <li>DOT</li> <li>Quantity limitations</li> </ul>	On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L
<ul> <li>IMDG</li> <li>Limited quantities (LQ)</li> <li>Excepted quantities (EQ)</li> </ul>	1L Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· IATA · Remarks:	When sold in quantities of less than or equal to 1 mL or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.
<ul> <li>Special precautions for user</li> <li>Hazard identification number (Kemler code)</li> <li>EMS Number:</li> <li>Stowage Category</li> <li>Stowage Code</li> </ul>	Warning: Flammable liquids : 33 F-E,S-D B SW2 Clear of living quarters.
· UN "Model Regulation":	UN 1648 ACETONITRILE SOLUTION, 3, II

# **15 Regulatory information**

• Safety, health and environmental regulations/legislation specific for the substance or mixture No further relevant information available.

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### · Section 355 (extremely hazardous substances):

None of the ingredients is listed.

### · Section 313 (Specific toxic chemical listings):

75-05-8 Acetonitrile

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TSCA (Toxic Substances Control Act):	
75-05-8 Acetonitrile	ACTIVE
Hazardous Air Pollutants	
75-05-8 Acetonitrile	
Chemicals known to cause cancer:	
None of the ingredients is listed.	
Chemicals known to cause reproductive toxicity for females:	
None of the ingredients is listed.	
Chemicals known to cause reproductive toxicity for males:	
None of the ingredients is listed.	
Chemicals known to cause developmental toxicity:	
None of the ingredients is listed.	
Carcinogenic categories	
EPA (Environmental Protection Agency)	
75-05-8 Acetonitrile	CBD, D
TLV (Threshold Limit Value)	
75-05-8 Acetonitrile	A4
NIOSH-Ca (National Institute for Occupational Safety and Health)	
None of the ingredients is listed.	
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.	

## **16 Other information**

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

- · Department issuing SDS: Environment protection department.
- · Contact: -
- Date of previous version 05/31/2022

 Date of preparation 02/05/2025 • Abbreviations and acronyms: IMDG: International Maritime Code for Dangerous Goods DOT: US Department of Transportation IATA: International Air Transport Association EINECS: European Inventory of Existing Commercial Chemical Substances ELINCS: European List of Notified Chemical Substances CAS: Chemical Abstracts Service (division of the American Chemical Society) NFPA: National Fire Protection Association (USA) HMIS: Hazardous Materials Identification System (USA) VOC: Volatile Organic Compounds (USA, EU) LC50: Lethal concentration, 50 percent LD50: Lethal dose, 50 percent PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative NIOSH: National Institute for Occupational Safety **OSHA: Occupational Safety & Health** 

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TLV: Threshold Limit Value PEL: Permissible Exposure Limit REL: Recommended Exposure Limit REL: Recommended Exposure Limit Flammable liquids 2: Flammable liquids – Category 2 Acute toxicity - oral 4: Acute toxicity – Category 4 Eye irritation 2A: Serious eye damage/eye irritation – Category 2A • \* Data compared to the previous version altered.

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