

## SAFETY DATA SHEET N,N-didesmethyl U-47700 (trifluoroacetate salt)

(CRM)

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according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 2015/830 and US OSHA HCS 2015

Section 1. Identification of the Substance/Mixture and of the Company/Undertaking

**1.1 Product Code:** 24289

Product Name: N,N-didesmethyl U-47700 (trifluoroacetate salt) (CRM)

**Synonyms:** trans-N-2-(aminocyclohexyl)-3,4-dichloro-N-methylbenzamide 2,2,2-trifluoroacetate;

nor-U-47700; N,N-didesethyl U-49900;

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

Relevant identified uses: For research use only, not for human or veterinary use.

1.3 Details of the Supplier of the Safety Data Sheet:

Company Name: Cayman Chemical Company

1180 E. Ellsworth Rd. Ann Arbor, MI 48108

Web site address: www.caymanchem.com

Information: Cayman Chemical Company +1 (734)971-3335

1.4 Emergency telephone number:

Emergency Contact: CHEMTREC Within USA and Canada: +1 (800)424-9300

CHEMTREC Outside USA and Canada: +1 (703)527-3887

#### Section 2. Hazards Identification

#### 2.1 Classification of the Substance or Mixture:

Flammable Liquids, Category 2

Acute Toxicity: Inhalation, Category 3
Acute Toxicity: Oral, Category 3
Acute Toxicity: Skin, Category 3

Specific Target Organ Toxicity (single exposure), Category 1

#### 2.2 Label Elements:







GHS Signal Word: Danger

#### **GHS Hazard Phrases:**

H225: Highly flammable liquid and vapor.

H301: Toxic if swallowed.

H311: Toxic in contact with skin.

H331: Toxic if inhaled.

H370: Causes damage to organs.

#### **GHS Precaution Phrases:**

P210: Keep away from {heat/sparks/open flames/hot surfaces}. - No smoking.

P260: Do not breathe {dust/fume/gas/mist/vapors/spray}.

P264: Wash {hands} thoroughly after handling.

P280: Wear {protective gloves/protective clothing/eye protection/face protection}.

#### **GHS** Response Phrases:

P301+310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P302+352: IF ON SKIN: Wash with plenty of soap and water.

P303+361+353: IF ON SKIN (or hair): Remove/take off immediately all contaminated clothing. Rinse skin with

water/shower.

P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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P307+311: IF exposed: Call a POISON CENTER or doctor/physician.

P311: Call a POISON CENTER or doctor/physician.

P330: Rinse mouth.

P361: Remove/Take off immediately all contaminated clothing.

P363: Wash contaminated clothing before reuse.

#### **GHS Storage and Disposal Phrases:**

Please refer to Section 7 for Storage and Section 13 for Disposal information.

2.3 Adverse Human Health Causes damage to organs {eyes}.

Effects and Symptoms: Material may be irritating to the mucous membranes and upper respiratory tract.

May be fatal or cause blindness if swallowed.

May cause eye, skin, or respiratory system irritation.

Toxic if inhaled, swallowed, or in contact with skin.

To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

## Section 3. Composition/Information on Ingredients

CAS#/ RTECS#	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
NA NA	N,N-didesmethyl U-47700 (trifluoroacetate salt)	0.1 %	NA NA	No data available.
67-56-1 PC1400000	Methanol 01-2119392409-28	99.9 %	200-659-6 603-001-00-X	Flam. Liq. 2: H225 Acute Tox.(O) 3: H301 Acute Tox.(D) 3: H311 Acute Tox.(I) 3: H331 STOT (SE) 1: H370

#### Section 4. First Aid Measures

#### 4.1 Description of First Aid

Measures:

In Case of Inhalation: Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel.

Get immediate medical attention.

In Case of Skin Contact: Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated

clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

In Case of Eye Contact: Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined

and tested by medical personnel.

In Case of Ingestion: Wash out mouth with water provided person is conscious. Never give anything by mouth to an

unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by

medical personnel.

4.2 Important Symptoms and Overexposure may cause: confusion, dermatitis, headache, drowsiness, dizziness, gastrointestinal

Effects, Both Acute and disturbance, optic nerve damage (blindness), nausea, unconsciousness, vomiting, visual

**Delayed:** disturbance, weakness.

May cause convulsions.

Once methanol is absorbed into the body, it is very slowly eliminated.



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Section 5. Fire Fighting Measures

5.1 Suitable Extinguishing Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.

Media: Use water spray to cool fire-exposed containers.

Unsuitable Extinguishing A solid water stream may be inefficient.

Media:

5.2 Flammable Properties andCan release vapors that form explosive mixtures at temperatures at or above the flashpoint.

Container explosion may occur under fire conditions.

Emits toxic fumes under fire conditions.

Sensitive to static discharge.

Vapors can travel to a source of ignition and flash back.

No data available.

Flash Pt: 11.00 C Method Used: Closed Cup

LEL: 6.0% at 25.0 C UEL: 36.0% at 25.0 C **Explosive Limits:** 

**Autoignition Pt:** 385.00 C

Fire Fighting Instructions: As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or 5.3

equivalent), and full protective gear to prevent contact with skin and eyes.

Note: Flammable as diluted in methanol.

#### Section 6. Accidental Release Measures

Avoid breathing vapors and provide adequate ventilation. 6.1 **Protective Precautions,** 

Protective Equipment and As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator,

and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves). **Emergency Procedures:** 

6.2 Take steps to avoid release into the environment, if safe to do so. **Environmental** 

Precautions:

6.3 Methods and Material For Contain spill and collect, as appropriate.

Containment and Cleaning Transfer to a chemical waste container for disposal in accordance with local regulations.

Up:

## Section 7. Handling and Storage

7.1 Precautions To Be Taken Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid prolonged or repeated exposure. in Handling:

Keep away from sources of ignition.

Take precautionary measures against static discharge.

7.2 Precautions To Be Taken Keep away from heat, sparks, and flame.

Keep container tightly closed. in Storing:

Store in accordance with information listed on the product insert.

#### Section 8. Exposure Controls/Personal Protection

#### 8.1 **Exposure Parameters:**

CAS#	Chemical Name	Jurisdiction	Recommended Exposure Limits	Notations
67-56-1	Methanol	ACGIH TLV	TLV: 200 ppm STEL: 250 ppm	
		Europe	TWA: 260 mg/m3 (200 ppm)	Skin Absorption
		France VL	TWA: 260 mg/m3 (200 ppm) STEL: 1300 mg/m3 (1000 ppm)	
		OSHA PELs	PEL: 200 ppm	
		Britain EH40	TWA: 266 mg/m3 (200 ppm) STEL: 333 mg/m3 (250 ppm)	Skin Absorption

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**Exposure Controls:** 

8.2.1 **Engineering Controls** Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne

levels below recommended exposure limits. (Ventilation etc.):

8.2.2 Personal protection equipment:

**Eye Protection:** Safety glasses

**Protective Gloves:** Compatible chemical-resistant gloves

Other Protective Clothing: Lab coat

**Respiratory Equipment** NIOSH approved respirator, as conditions warrant.

(Specify Type):

Work/Hygienic/Maintenan Do not take internally.

Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower. ce Practices:

Wash thoroughly after handling.

No data available.

## Section 9. Physical and Chemical Properties

9.1 Information on Basic Physical and Chemical Properties

> [X] Liquid **Physical States:** [ ] Gas [ ] Solid A 1 mg/ml solution in methanol Appearance and Odor:

pH: No data. **Melting Point:** No data. No data. **Boiling Point:** 

Flash Pt: 11.00 C Method Used: Closed Cup

**Evaporation Rate:** No data.

Flammability (solid, gas): No data available.

LEL: 6.0% **Explosive Limits:** at 25.0 C UEL: 36.0% at 25.0 C

Vapor Pressure (vs. Air or mm 96 MM\_HG at 20.0 C

Hg):

Vapor Density (vs. Air = 1): No data. Specific Gravity (Water = 1): No data. No data. Solubility in Water: **Octanol/Water Partition** No data.

Coefficient:

385.00 C **Autoignition Pt:** No data. **Decomposition Temperature:** Viscosity: No data.

9.2 **Other Information** 

> **Percent Volatile:** No data.

Molecular Formula & Weight: C14H18Cl2N2O • XCF3COOH 301.2



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## Section 10. Stability and Reactivity

**10.1 Reactivity:** No data available.

**10.2 Stability:** Unstable [ ] Stable [ X ]

**10.3 Stability Note(s):** Stable if stored in accordance with information listed on the product insert.

Polymerization: Will occur [ ] Will not occur [ X ]

**10.4 Conditions To Avoid:** heat, flames, and sparks

10.5 Incompatibility - Materials acids

To Avoid: acid anhydrides

acid chlorides
alkali metals
oxidizing agents
reducing agents
carbon dioxide

10.6 Hazardous

Decomposition or carbon monoxide

Byproducts:

#### Section 11. Toxicological Information

**11.1** Information on The toxicological effects of this product have not been thoroughly studied.

Toxicological Effects: Methanol - Toxicity Data: Oral LD50 (rat): 5,600 mg/kg; Oral LD50 (rabbit): 14,200 mg/kg; Oral

LDLO (man): 6422 mg/kg; Intraperitoneal LD50 (mouse): 10765 mg/kg;

Inhalation LC50 (rat): 64,000 ppm (4h); Inhalation LC50 (mouse): 61,100 ppm (134 m); Skin LD50

(rabbit): 15,800 mg/kg; Oral LDLO (human): 143 mg/kg;

Methanol - Irritation Data: Skin (rabbit): 20 mg (24h) moderate; Eyes (rabbit): 40 mg moderate;

Eyes (rabbit): 100 mg (24h) moderate;

**Chronic Toxicological** 

Effects:

Methanol - Investigated as a drug, mutagen, primary irritant, reproductive effector, and tumorigen. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here.

See actual entry in RTECS for complete information.

Methanol RTECS Number: PC1400000

Carcinogenicity: NTP? No IARC Monographs? No OSHA Regulated? No

CAS#	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
NA	N,N-didesmethyl U-47700 (trifluoroacetate salt)	n.a.	n.a.	n.a.	n.a.
67-56-1	Methanol	n.a.	n.a.	n.a.	n.a.

## Section 12. Ecological Information

**12.1 Toxicity:** Avoid release into the environment.

Runoff from fire control or dilution water may cause pollution.

**12.2 Persistence and** No data available.

Degradability:

**12.3** Bioaccumulative No data available.

Potential:

**12.4 Mobility in Soil:** No data available.

**12.5** Results of PBT and vPvB No data available.

assessment:

**12.6** Other adverse effects: No data available.

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## Section 13. Disposal Considerations

**13.1 Waste Disposal Method:** Dispose in accordance with local, state, and federal regulations.

## Section 14. Transport Information

#### 14.1 LAND TRANSPORT (US DOT):

**DOT Proper Shipping Name:** Methanol Solution

**DOT Hazard Class:** 3 (6.1) FLAMMABLE LIQUID, POISON

UN/NA Number: UN1230 Packing Group: II





#### 14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name: Methanol Solution

UN Number: 1230 Packing Group: II

Hazard Class: 3 (6.1) - FLAMMABLE LIQUID,

**POISON** 

#### 14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Methanol Solution

UN Number: 1230 Packing Group: II

Hazard Class: 3 (6.1) - FLAMMABLE LIQUID, IATA Classification: 3, 6.1

**POISON** 

Additional Transport Transport in accordance with local, state, and federal regulations.

Information: 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.

## Section 15. Regulatory Information

#### EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists

CAS#	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
NA	N,N-didesmethyl U-47700 (trifluoroacetate salt)	No	No	No
67-56-1	Methanol	No	Yes 5000 LB	Yes
CAS#	Hazardous Components (Chemical Name)	Other US EPA or State Lists		
NA	N,N-didesmethyl U-47700 (trifluoroacetate salt)	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA		

CAS#	Hazardous Components (Chemical Name)	Other US EPA or State Lists
NA	N,N-didesmethyl U-47700 (trifluoroacetate salt)	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA
		PROP.65: No
67-56-1	Methanol	CAA HAP,ODC: HAP: VHAP; CWA NPDES: No; TSCA: Yes - Inventory; CA PROP.65: Yes: RDTox.
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Statement:

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Regulatory Information

This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC)

No.1272/2008.

Section 16. Other Information

**Revision Date:** 09/09/2019

Additional Information About

No data available.

This Product:

Company Policy or Disclaimer: DISCLAIMER: This information is believed to be accurate and represents the best information

currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for

their particular purposes.