

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

Date of issue: 18/01/2018 Revision date: : Version: 1.0

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

1.1. Product identifier

Product form : Mixture

Product name : SOM01.1 Ketone Deuterated Monitoring Compounds

Product code : AL0-101664
Product group : Trade product

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

1.2.1. Relevant identified uses

Main use category : Laboratory Use Industrial/Professional use spec : Industrial

For professional use only

Use of the substance/mixture : Certified reference material for laboratory use only

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Phenova

6390 Joyce Dr. Suite 100 80403 Golden, CO - United States T 1-866-942-2978 - F 1-866-283-0269 info@phenova.com - www.phenova.com

1.4. Emergency telephone number

Emergency number : ChemTel Assistance (US/Canada) 1-800-255-3924

ChemTel Assistance (International) +1 813-248-0585

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

 Flam. Liq. 2
 H225

 Acute Tox. 3 (Oral)
 H301

 Acute Tox. 3 (Dermal)
 H311

 STOT SE 1
 H370

Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Not classified

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP)



GHS02





GHS06

GHS08

Signal word (CLP) : Danger

Hazard statements (CLP) : H225 - Highly flammable liquid and vapor

H301+H311 - Toxic if swallowed or in contact with skin

H370 - Causes damage to organs

Precautionary statements (CLP) : P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No

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smoking

P233 - Keep container tightly closed

P260 - Do not breathe dust/fume/gas/mist/vapors/spray P270 - Do not eat, drink or smoke when using this product

P280 - Wear protective gloves/protective clothing/eye protection/face protection P301+P330+P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting

P303+P361+P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing.

Rinse skin with water

P308+P313 - IF exposed or concerned: Get medical advice/attention

P361+P364 - Take off immediately all contaminated clothing and wash it before reuse

P370+P378 - In case of fire: Use media other than water to extinguish

P403+P235 - Store in a well-ventilated place. Keep cool

P501 - Dispose of contents/container to hazardous or special waste collection point, in

accordance with local, regional, national and/or international regulation

No labeling applicable

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1 Substances

Not applicable

3.2. Mixtures

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
methanol-d1 (Component)	(CAS No) 1455-13-6 (EC-No.) 215-933-0 (EC index no) 603-001-00-X	89.9	Flam. Liq. 2, H225 Acute Tox. 3 (Inhalation), H331 Acute Tox. 3 (Dermal), H311 Acute Tox. 3 (Oral), H301 STOT SE 1, H370
Name	Product identifier	Specific o	concentration limits
methanol-d1 (Component)	(CAS No) 1455-13-6 (EC-No.) 215-933-0 (EC index no) 603-001-00-X		0) STOT SE 2, H371 TOT SE 1, H370

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Never give anything by mouth to an unconscious person. Call a POISON CENTER or

doctor/physician. IF exposed or concerned: Get medical advice/attention.

First-aid measures after inhalation

: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

First-aid measures after skin contact

Rinse skin with water/shower. Remove/Take off immediately all contaminated clothing. Immediately call a poison center or doctor/physician. Wash with plenty of soap and water.

Wash contaminated clothing before reuse.

First-aid measures after eye contact

: Remove contact lenses, if present and easy to do. Continue rinsing. Rinse cautiously with water for several minutes. Obtain medical attention if pain, blinking or redness persists.

First-aid measures after ingestion

Rinse mouth. Do NOT induce vomiting. Obtain emergency medical attention. Immediately call a poison center or doctor/physician.

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

Symptoms/effects after skin contact

: Repeated exposure to this material can result in absorption through skin causing significant

health hazard. Toxic in contact with skin.

Symptoms/effects after ingestion

Toxic if swallowed. Swallowing a small quantity of this material will result in serious health

hazard

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Use extinguishing media appropriate for surrounding fire.

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Highly flammable liquid and vapor.

Explosion hazard : May form flammable/explosive vapor-air mixture.

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5.3. Advice for firefighters

Firefighting instructions : Use water spray or fog for cooling exposed containers. Exercise caution when fighting any

chemical fire. Prevent fire-fighting water from entering environment.

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection. Avoid breathing dust/fume/gas/mist/vapors/spray.

Emergency procedures : Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Take up in absorbent material. Collect spillage.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.

Precautions for safe handling : Wash hands and other exposed areas with mild soap and water before eating, drinking or

smoking and when leaving work. Provide good ventilation in process area to prevent formation of vapor. No open flames. No smoking. Use only non-sparking tools.

Hygiene measures : Do not eat, drink or smoke when using this product. Gently wash with plenty of soap and water.

Remove/Take off immediately all contaminated clothing. Wash contaminated clothing before reuse

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Proper grounding procedures to avoid static electricity should be followed. Ground/bond

container and receiving equipment.

Storage conditions : Keep in fireproof place. Keep container tightly closed. Keep container tightly closed and in a

well-ventilated place. Keep away from any flames or sparking source.

Incompatible materials : Direct sunlight. Heat sources.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls : Either local exhaust or general room ventilation is usually required.

Personal protective equipment : Avoid all unnecessary exposure. Gloves. Protective clothing. Protective goggles. Safety

glasses.



Hand protection : Wear chemically resistant protective gloves. Wear suitable gloves resistant to chemical

Eye protection : Chemical goggles or safety glasses. Safety glasses.

Skin and body protection : Wear chemically protective gloves, lab coat or apron to prevent prolonged or repeated skin

contact.

Respiratory protection : Where exposure through inhalation may occur from use, respiratory protection equipment is

recommended.

Other information : Do not eat, drink or smoke during use.

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SECTION 9: Physical and chemical properties

1. Information on basic physical and chemical properties

Physical state : Liquid Color : Colorless. Odor : characteristic No data available pΗ Melting point : No data available Freezing point : No data available : No data available Boiling point Flash point : No data available : No data available Auto-ignition temperature Decomposition temperature : No data available

Flammability (solid, gas) : Highly flammable liquid and vapor

Relative density : No data available Solubility : No data available Explosive properties : No data available Oxidizing properties : No data available Explosion limits : No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Highly flammable liquid and vapor. May form flammable/explosive vapor-air mixture.

10.3. Possibility of hazardous reactions

Not established.

10.4. Conditions to avoid

Direct sunlight. Extremely high or low temperatures. Open flame.

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

May release flammable gases.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Toxic if swallowed. Dermal: Toxic in contact with skin.

SOM01.1 Ketone Deuterated Monitoring Comp	pounds
ATE CLP (oral)	111.234705228 mg/kg body weight
ATE CLP (dermal)	333.7041156841 mg/kg body weight
methanol-d1 (1455-13-6)	
ATE CLP (oral)	100 mg/kg body weight
ATE CLP (dermal)	300 mg/kg body weight
ATE CLP (gases)	700 ppmV/4h
ATE CLP (vapors)	3 mg/l/4h
ATE CLP (dust, mist)	0.5 mg/l/4h

Skin corrosion/irritation : Not classified

Based on available data, the classification criteria are not met

Serious eye damage/irritation : Not classified

Based on available data, the classification criteria are not met

Respiratory or skin sensitization : Not classified

Based on available data, the classification criteria are not met

Germ cell mutagenicity : Not classified

Based on available data, the classification criteria are not met

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Carcinogenicity : Not classified

Based on available data, the classification criteria are not met

May cause cancer

Reproductive toxicity : Not classified

Based on available data, the classification criteria are not met

Specific target organ toxicity – single exposure : Causes damage to organs.

Specific target organ toxicity – repeated : Not classified

exposure

Based on available data, the classification criteria are not met

Aspiration hazard : Not classified

Based on available data, the classification criteria are not met

Potential Adverse human health effects and

symptoms

: Toxic if swallowed. Toxic in contact with skin.

SECTION 12: Ecological information

12.1. Toxicity

methanol-d1 (1455-13-6)	
LC50 fish 1	10800 mg/l (96 h, Salmo gairdneri)
EC50 Daphnia 1	24500 mg/l (48 h, Daphnia magna)

12.2. Persistence and degradability

SOM01.1 Ketone Deuterated Monitoring	Compounds
Persistence and degradability	Not established.
methanol-d1 (1455-13-6)	
Persistence and degradability	Biodegradable in the soil. Readily biodegradable in water.
Biochemical oxygen demand (BOD)	0.6 - 1.1 g O ₂ /g substance
Chemical oxygen demand (COD)	1.42 g O₂/g substance
ThOD	1.5 g O ₂ /g substance
BOD (% of ThOD)	0.40 - 0.73

12.3. Bioaccumulative potential

SOM01.1 Ketone Deuterated Monitoring Comp	pounds
Bioaccumulative potential	Not established.
methanol-d1 (1455-13-6)	
BCF fish 1	< 10 (Leuciscus idus, Non deuterium form)
Log Pow	-0.820.66
Bioaccumulative potential	Not bioaccumulative.

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Additional information : Avoid release to the environment

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Additional information : Handle empty containers with care because residual vapors are flammable.

Ecology - waste materials : Avoid release to the environment. Hazardous waste due to toxicity.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

14.1. UN number

 UN-No. (ADR)
 : 1992

 UN-No. (IATA)
 : 1992

 UN-No. (IMDG)
 : 1992

 UN-No. (ADN)
 : 1992

14.2. UN proper shipping name

Proper Shipping Name (ADR) : FLAMMABLE LIQUID, TOXIC, N.O.S.

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Proper Shipping Name (IATA) : Flammable liquid, toxic, n.o.s.

Proper Shipping Name (IMDG) : FLAMMABLE LIQUID, TOXIC, N.O.S.

Proper Shipping Name (ADN) : FLAMMABLE LIQUID, TOXIC, N.O.S.

Transport document description (ADR) : UN 1992 FLAMMABLE LIQUID, TOXIC, N.O.S., 3 (6.1), II, (D/E)

14.3. Packing group

Class (ADR) : 3 : FT1 Classification code (ADR) Class (IATA) : 3 Class (IMDG) : 3 : 3 Class (ADN) Classification code (ADN) : FT1 Subsidiary risks (ADR) : 6.1 Subsidiary risks (IMDG) : 6.1 Hazard labels (ADR) : 3, 6.1



Hazard labels (IATA) : 3, 6.1



Hazard labels (IMDG) : 3, 6.1



Hazard labels (ADN) : 3, 6.1



14.4. Packing group

Packing group (ADR) : II
Packing group (IATA) : II
Packing group (IMDG) : II
Packing group (ADN) : II

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

14.6.1. Overland transport

Hazard identification number (Kemler No.) : 336 Classification code (ADR) : FT1

Orange plates

336 1992

Special provision (ADR) : 274

Transport category (ADR) : 2

Tunnel restriction code (ADR) : D/E

Limited quantities (ADR) : 11

Excepted quantities (ADR) : E2

14.6.2. Transport by sea

Special provision (IMDG) : 274

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Limited quantities (IMDG) : 1L Excepted quantities (IMDG) : E2 Packing instructions (IMDG) : P001 IBC packing instructions (IMDG) : IBC02 Tank instructions (IMDG) : T7 : TP2, TP13 Tank special provisions (IMDG) : F-E EmS-No. (Fire) : S-D EmS-No. (Spillage) Stowage category (IMDG) : B

Properties and observations (IMDG) : Flammable toxic liquid which is not specified by name in this class or, on account of its

characteristics, in some other class. Toxic if swallowed, by skin contact or by inhalation.

14.6.3. Air transport

CAO packing instructions (IATA) : 364 CAO max net quantity (IATA) : 60L PCA packing instructions (IATA) : 352 PCA Limited quantities (IATA) : Y341 PCA limited quantity max net quantity (IATA) : 1L PCA max net quantity (IATA) : 1L PCA Excepted quantities (IATA) : E2 Special provision (IATA) : A3 ERG code (IATA) : 3HP

14.6.4. Inland waterway transport

Special provision (ADN) : 274, 802
Limited quantities (ADN) : 1 L

Excepted quantities (ADN) : E2

Carriage permitted (ADN) : T

Equipment required (ADN) : PP, EP, EX, TOX, A

Ventilation (ADN) : VE01, VE02

Number of blue cones/lights (ADN) : 2
Carriage prohibited (ADN) : No

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

Contains no REACH substances with Annex XVII restrictions

Contains no REACH candidate substance

Contains no REACH Annex XIV substances.

15.1.2. National regulations

Germany

Water hazard class (WGK) : 3 - strongly hazardous to water

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

SECTION 16: Other information

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE

COUNCIL of 16 December 2008 on classification, labeling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending

Regulation (EC) No 1907/2006.

Other information : None.

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