

Beta Ionone - dsm-firmenich

Version 1.0

Revision Date 10/08/2014

Print Date 05/07/2015

**SECTION 1. PRODUCT AND COMPANY IDENTIFICATION**

Product name Substance : Beta-Ionone-dsm-firmenich  
 name : (E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one  
 CAS-No. : 79-77-6

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

Use of the Sub- : Ingredient for fragrances  
 stance/Mixture

**1.3 Details of the supplier of the safety data sheet**

Company : DSM Nutritional Products Ltd.  
 PO Box 2676  
 CH-4002 Basel  
 Telephone : +41618158888  
 Telefax : +41618157253  
 E-mail address Respon- : sds.nutritionalproducts@dsm.com  
 sible/issuing person

**1.4 Emergency telephone number**

+41 62 866 2314

**SECTION 2. HAZARDS IDENTIFICATION****Emergency Overview**

Appearance	oily liquid
Colour	pale yellow
Odour	characteristic

**GHS Classification**

Not a hazardous substance or mixture.

**GHS Label element**

Not a hazardous substance or mixture.

**Potential Health Effects**

Aggravated Medical Condi- : None known.  
 tion

Symptoms of Overexposure : No specific symptoms known.

**Carcinogenicity:****IARC**

No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

**ACGIH**

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

**OSHA**

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

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**NTP** No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

**Additional hazards and advice**

In case of extensive air contact (e.g. soaked rags, moistened clothes) an exothermic autooxidation (self-ignition) is possible.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Synonyms 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (E)-

Brief description of the product Substance

Molecular formula C<sub>13</sub>H<sub>20</sub>O

**Hazardous components** No

hazardous ingredients

**Further ingredients**

Component	CAS-No.	Weight percent
(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-77-6	90 - 100

**SECTION 4. FIRST AID MEASURES**

General advice : No hazards which require special first aid measures.

If inhaled : Move to fresh air.  
Consult a physician after significant exposure.

In case of skin contact : Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water.

In case of eye contact : Flush eyes with water as a precaution. Remove contact lenses.  
Protect unharmed eye.  
Keep eye wide open while rinsing.  
If eye irritation persists, consult a specialist.

If swallowed : Clean mouth with water and drink afterwards plenty of water.  
Do not give milk or alcoholic beverages.  
Never give anything by mouth to an unconscious person. If symptoms persist, call a physician.

Most important symptoms and effects, both acute and delayed : No specific symptoms known.

Notes to physician : Treat symptomatically.

**SECTION 5. FIREFIGHTING MEASURES****Flammable properties**

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Flash point : 259 °F (126 °C)  
Method: Tested according to Directive 92/69/EEC.

Ignition temperature : 273 °C (Tested according to Directive 92/69/EEC.)

Lower explosion limit : not determined

Upper explosion limit : not determined

**Fire fighting**

Suitable extinguishing media : Alcohol-resistant foam  
Dry chemical  
Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media : High volume water jet

Further information : Collect contaminated fire extinguishing water separately. This must not be discharged into drains.  
Fire residues and contaminated fire extinguishing water must be disposed of in accordance with local regulations.

**Protective equipment and precautions for firefighters**

Specific hazards during fire-fighting : Do not allow run-off from fire fighting to enter drains or water courses.

Special protective equipment for firefighters : In the event of fire, wear self-contained breathing apparatus.

**SECTION 6. ACCIDENTAL RELEASE MEASURES**

Personal precautions, protective equipment and emergency procedures : Use personal protective equipment. Ensure adequate ventilation.

Environmental precautions : Do not flush into surface water or sanitary sewer system.  
Prevent further leakage or spillage if safe to do so.  
If the product contaminates rivers and lakes or drains inform respective authorities.

Methods and materials for containment and cleaning up : Wipe up with absorbent material (e.g. cloth, fleece). Keep in suitable, closed containers for disposal.

**SECTION 7. HANDLING AND STORAGE**

Advice on safe handling : For personal protection see section 8.  
Dispose of rinse water in accordance with local and national regulations.  
handle under inert gas

Advice on protection against fire and explosion : Take necessary action to avoid static electricity discharge.  
Product will burn under fire conditions.

Conditions for safe storage : Protect against light.

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Protect from humidity. Keep under inert gas.

Keep container tightly closed and dry.  
Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage temperature : &lt; 77 °F (&lt; 25 °C)

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

**Personal protective equipment**

Respiratory protection : In case of mist, spray or aerosol exposure wear suitable personal respiratory protection and protective suit.

In the case of vapour formation use a respirator with an approved filter.

Hand protection : Glove material: for example nitrile rubber

Eye protection : Safety glasses with side-shields

Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice.  
Wash hands before breaks and at the end of workday.**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES****9.1 Information on basic physical and chemical properties**

Appearance : oily liquid  
Colour : pale yellow  
Odour : characteristic  
Odour Threshold : No information available.  
pH : No data available  
Melting point/range : < -20 °C  
Boiling point/boiling range : 267.1 °C (at 1,013 hPa)  
Flash point : 126 °C (Tested according to Directive 92/69/EEC.)  
Evaporation rate : not determined  
Lower explosion limit : not determined  
Upper explosion limit : not determined  
Vapour pressure : 0.072 hPa (at 25 °C)  
Relative vapour density : not determined

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Density	: 0.9447 g/cm <sup>3</sup> (at 20 °C)
Water solubility	: 0.11 g/l (20 °C; OECD Test Guideline 105) practically insoluble
Solubility in other solvents	: Ethanol: soluble Diethylether: soluble Dichloromethane: soluble
Partition coefficient: n-octanol/water	: log Pow 4 (25 °C)
Ignition temperature Thermal decomposition	: 273 °C (Tested according to Directive 92/69/EEC.)
Viscosity, dynamic	: No data available
Explosive properties	: 11.2 mPa.s (at 20 °C, OECD Test Guideline 114)
Oxidizing properties	: Not explosive
Oxidizing properties	: Not oxidizing

## 9.2 Other information

Molecular weight	192.3 g/mol
Surface tension	ca. 27 mN/m (20 °C)

## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: No hazards to be specially mentioned.
Chemical stability	: Stable under recommended storage conditions.
Possibility of hazardous reactions	: In case of extensive air contact (e.g. soaked rags, moistened clothes) an exothermic autooxidation (self-ignition) is possible.
Conditions to avoid	: Heat. Exposure to air.
Incompatible materials	: Strong acids and strong bases Oxidizing agents
Hazardous decomposition products	: No decomposition if used as directed.

## SECTION 11. TOXICOLOGICAL INFORMATION

Acute oral toxicity	: LD50 (Rat): > 4,000 mg/kg
Acute dermal toxicity	: LD50 (Rat, male and female): > 2,000 mg/kg tested with an isomer mixture (OECD Test Guideline 402)
Skin irritation	: No skin irritation (Rabbit, OECD Test Guideline 404) : No skin irritation (human)

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tested with an isomer mixture

Eye irritation	: No eye irritation (Rabbit, OECD Test Guideline 405)
Sensitisation	: Does not cause skin sensitisation. (Guinea pig, OECD Test Guideline 406) tested with the racemate
Carcinogenicity	: No indication for carcinogenicity known.
Genotoxicity in vitro	: negative (Ames test) tested with an isomer mixture : positive (Chromosome aberration test in vitro) Test performed using a similar product.
Genotoxicity in vivo	: not genotoxic (Chromosome aberration test in vitro, Mouse, Intraperitoneal injection, OECD Test Guideline 474)
Reproductive toxicity	: NOAEL: 720 mg/kg bw/d (Rat, males, Oral, OECD Test Guideline 408)
Teratogenicity	: NOAEL: 400 mg/kg bw/d (Rat, Oral, OECD Test Guideline 414) : NOAEL: 50 mg/kg bw/d (Rabbit, Oral, OECD Test Guideline 414)
STOT - single exposure (Acute exposure)	: The substance or mixture is not classified as specific target organ toxicant, single exposure.
STOT - repeated exposure	: NOAEL (Oral, Rat, male) : 71.8 mg/kg body weight Sub-chronic toxicity study (90-day) (OECD Test Guideline 408)
Experience with human exposure	: May cause sensitisation of susceptible persons., (Cases have been reported rarely.)
Aspiration toxicity	: No aspiration toxicity classification

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**SECTION 12. ECOLOGICAL INFORMATION**
**Toxicity**

Toxicity to fish	: Pimephales promelas (fathead minnow) LC50 (96 h) 5.09 mg/l
Toxicity to daphnia and other aquatic invertebrates	: Daphnia magna (Water flea) EC50 (48 h) 4.03 mg/l (OECD Test Guideline 202)

# SAFETY DATA SHEET



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- Toxicity to algae : Desmodesmus subspicatus (green algae)  
EC50 (72 h) 21.2 mg/l  
(DIN 38412)
- Toxicity to bacteria : activated sludge  
EC50 (3 h) 100 - 200 mg/l  
(OECD Test Guideline 209)
- Ecotoxicology Assessment
- Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

- Persistence and degradability** : Readily biodegradable.  
70 - 80 % (28 d)  
(Tested according to Annex V of Directive 67/548/EEC.)
- Biodegradability

### Bioaccumulative potential

- Partition coefficient: n-octanol/water : log Pow 4 ( 25 °C )

### Mobility in soil

- Adsorption/Soil : log Koc 2.8 (calculated value)  
Mobile in soils
- Distribution among environmental compartments
- Surface tension : ca. 27 mN/m ( 20 °C )

### Results of PBT and vPvB assessment

- Assessment : The substance does not fulfill the PBT criteria. :  
The substance does not fulfill the vPvB criteria.

### Other adverse effects

- Regulation 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
- Remarks This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Additional ecological information- : Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

- Waste from residues Organic materials (e.g. rags, paper, wood) which are soaked with this product can heat up and catch fire in the presence of air, even at room temperature: store in the absence of air (e.g. in water) and send it for incineration (or dispose of in accordance with local regulations).  
Beta Ionone - dsm-firmenich Discharge into the environment must be avoided.  
Do not contaminate ponds, waterways or ditches with chemi-

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cal or used container.

Do not dispose of waste into sewer.

Offer surplus and non-recyclable solutions to a licensed disposal company.

User must determine if any wastes generated exhibit hazardous characteristics as per 40 CFR Part 261 or other national / local legislation.

Contaminated packaging

Dispose of as unused product.

Do not re-use empty containers.

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**SECTION 14. TRANSPORT INFORMATION**
**International Regulation****IATA-DGR**

UN/ID No.

: UN 3082

Proper shipping name

: Environmentally hazardous substance, liquid, n.o.s.  
((E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Class

: 9

Packing group

: III

Labels

: Miscellaneous Dangerous Goods

Packing instruction (cargo aircraft)

: 964

Packing instruction (passenger aircraft)

: 964

**IMDG-Code**

UN number

: UN 3082

Proper shipping name

: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,  
N.O.S.  
((E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Class

: 9

Packing group

: III

Labels

: 9

EmS Code

: F-A, S-F

Marine pollutant

: yes

**Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code** Not applicable for product as supplied.

**National Regulations****49 CFR**

UN/ID/NA number

: UN 3082

Proper shipping name

: Environmentally hazardous substances, liquid, n.o.s.  
((E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Class

: 9

Packing group

: III

Labels

: CLASS 9

ERG Code

: 171

Marine pollutant

: yes ((E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Remarks

: No additional requirements.

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**SECTION 15. REGULATORY INFORMATION**

**TSCA list** : Not relevant  
 Not relevant

**EPCRA - Emergency Planning and Community Right-to-Know Act****CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 311/312 Hazards** : No SARA Hazards

**SARA 302** : No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**Clean Air Act**

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 12 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

**Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

**Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know**

(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-77-6	90 - 100 %
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**New Jersey Right To Know**

(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-77-6	90 - 100 %
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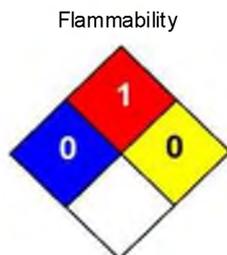
**The components of this product are reported in the following inventories:**

**TSCA** : On TSCA Inventory

## SECTION 16. OTHER INFORMATION

## Further information

## NFPA:



Special hazard.

## HMIS III:

HEALTH	1
FLAMMABILITY	1
PHYSICAL HAZARD	0

0 = not significant, 1 = Slight,  
2 = Moderate, 3 = High  
4 = Extreme, \* = Chronic

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

**Abbreviations:** ACGIH = American Conference of Governmental Industrial Hygienists. CERCLA = Comprehensive Environmental Response, Compensation and Liability Act. CFR = Code of Federal Regulations. CPR = Controlled Products Regulations. DSL = Canadian Domestic Substance List. DOT = Department of Transportation. EINECS = European Inventory of New and Existing Chemical Substances. EPA = Environmental Protection Agency. HCS = Hazardous Communication Standard. HEPA = High Efficiency Particulate Air. HMIS = Hazardous Material Identification System. IARC = International Agency for Research on Cancer. IATA = International Air Transport Association. IMDG = International Maritime Dangerous Good. NFPA = National Fire Protection Association. NIOSH = National Institute of Occupational Safety and Health. NJTSR = New Jersey Trade Secret Registry. NTP = National Toxicology Program. OSHA = Occupational Safety and Health Administration. SARA = Superfund Amendments and Reauthorization Act. TDG = Transportation of Dangerous Goods. TLV = Threshold Limit Value. TSCA = Toxic Substance Control Act. WHMIS = Workplace Hazardous Materials Information System.