

**SECTION 1. PRODUCT AND COMPANY IDENTIFICATION**

Product name : Isonaline 95  
 Substance name : 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one  
 CAS-No. : 127-51-5

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

Use of the Sub- : Raw material, 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**

<b>CAUTION</b>	
Appearance	oily liquid
Colour	pale yellow
Odour	characteristic

**GHS Classification**

Skin irritation : Category 2  
 Eye irritation : Category 2A

**GHS Label element**

Hazard pictograms : 

Signal word : Warning

Hazard statements : H315 Causes skin irritation.  
 H319 Causes serious eye irritation.

Precautionary statements : **Prevention:**  
 P264 Wash skin thoroughly after handling.  
 P280 Wear protective gloves/ eye protection/ face protection.  
**Response:**  
 P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
 P305 + P351 + P338 IF IN EYES: Rinse cautiously with water

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for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P332 + P313 If skin irritation occurs: Get medical advice/ attention.

P337 + P313 If eye irritation persists: Get medical advice/ attention.

P362 Take off contaminated clothing and wash before reuse.

**Potential Health Effects**

Primary Routes of Entry : Skin Absorption

Skin : May cause skin irritation.

Eyes : May cause eye irritation.

Aggravated Medical Condition : None known.

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.

**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**

None known.

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

Brief description of the product : Mixture of isomers

Molecular formula : C14-H22-O

**Hazardous components**

Component	CAS-No.	Weight percent
3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5	90 - 100
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-89-0	5 - 10
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	7779-30-8	5 - 10

**SECTION 4. FIRST AID MEASURES**

- General advice : Move out of dangerous area.  
Show this safety data sheet to the doctor in attendance.
- 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.  
If symptoms persist, call a physician.
- In case of eye contact : Immediately flush eye(s) with plenty of water.  
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.  
Obtain medical attention.
- Most important symptoms and effects, both acute and delayed : No specific symptoms known.
- Notes to physician : Treat symptomatically.

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

- Flash point : 223 °F (106 °C)  
Method: DIN 51758
- Ignition temperature : 270 °C (DIN 51794)
- Lower explosion limit : not determined
- Upper explosion limit : not determined
- Flammability (solid, gas) : The substance or mixture is not classified as pyrophoric., The substance or mixture does not emit flammable gases in contact with water.

**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.

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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 : Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust).  
Keep in suitable, closed containers for disposal.

**SECTION 7. HANDLING AND STORAGE**

Advice on safe handling : Avoid contact with skin and eyes.  
For personal protection see section 8.  
Dispose of rinse water in accordance with local and national regulations.  
Smoking, eating and drinking should be prohibited in the application area.

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

Storage temperature : < 77 °F (< 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 the case of vapour formation use a respirator with an approved filter.

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	In case of mist, spray or aerosol exposure wear suitable personal respiratory protection and protective suit.
Hand protection	: Glove material: for example nitrile rubber  Glove material: butyl-rubber  Consider the hazard characteristics of this product and any special workplace conditions when selecting the appropriate type of protective gloves.
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
Boiling point/boiling range	: 266.2 °C (at 1,013 hPa) 162.2 °C (at 53.3 hPa) 126.5 °C (at 13.3 hPa)
Flash point	: 106 °C (DIN 51758)
Evaporation rate	: not determined
Flammability (solid, gas)	: The substance or mixture is not classified as pyrophoric., The substance or mixture does not emit flammable gases in contact with water.
Lower explosion limit	: not determined
Upper explosion limit	: not determined
Vapour pressure	: not determined
Relative vapour density	: not determined
Density	: 0.93 g/cm <sup>3</sup> (at 20 °C)
Water solubility	: practically insoluble ca. 16 mg/l (20 °C; OECD Test Guideline 105) Test performed using a similar product.
Solubility in other solvents	: various organic solvents: soluble
Partition coefficient: n-octanol/water	: log Pow ca. 4.5 - 5.0 ( 25 °C; OECD Test Guideline 117) Test performed using a similar product.

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Ignition temperature : 270 °C (DIN 51794)  
Thermal decomposition : Not relevant  
Explosive properties : Not explosive  
Oxidizing properties : Not oxidizing

**9.2 Other information**

No data available

**SECTION 10. STABILITY AND REACTIVITY**

Reactivity : No hazards to be specially mentioned.  
Chemical stability : Stable under recommended storage conditions.  
Possibility of hazardous reactions : Possible incompatibility with materials listed under section 10.5.  
Conditions to avoid : Heat.  
Incompatible materials : Strong acids and strong bases  
Strong oxidizing agents  
Hazardous decomposition products : No decomposition if used as directed.

**SECTION 11. TOXICOLOGICAL INFORMATION**

Acute oral toxicity : LD50 (Rat): > 5,000 mg/kg  
Acute dermal toxicity : LD50 (Rabbit): > 5,000 mg/kg  
Skin irritation : Moderate skin irritation (Rabbit)  
Eye irritation : May irritate eyes.  
Sensitisation : Did not cause sensitization. (Guinea pig)  
: no photoallergenic skin reaction (Guinea pig)  
Test performed using a similar product.  
Carcinogenicity : No indication for carcinogenicity known.  
Genotoxicity in vitro : not mutagenic (Ames test, OECD Test Guideline 471)  
Test performed using a similar product.  
Genotoxicity in vivo : not genotoxic (In vivo micronucleus test, Mouse)

	: Test performed using a similar product.
Reproductive toxicity	: No indication for adverse effects on fertility known.
Teratogenicity	: No indication for teratogenicity known.
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) : 30 mg/kg bw/d Sub-chronic toxicity study (90-day) Information refers to the main component. (OECD Test Guideline 408) : LOAEL (Oral, Rat, male) : 500 mg/kg bw/d Sub-chronic toxicity study (90-day) Information refers to the main component. (OECD Test Guideline 408)
Further information	: The product passes into and partly through the skin of rats and pigs.  : May cause irritation of respiratory tract.
Aspiration toxicity	: No aspiration toxicity classification

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

Toxicity to fish	: Danio rerio (zebra fish) LC50 (96 h) ca. 2.3 mg/l Test performed using a similar product. (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	: Daphnia magna (Water flea) EC50 (48 h) 3.7 mg/l Test performed using a similar product. (OECD Test Guideline 202)
Toxicity to algae	: Desmodesmus subspicatus (green algae) EC50 (72 h) > 9.42 mg/l Test performed using a similar product. (OECD Test Guideline 201)
Toxicity to bacteria	: activated sludge EC50 (1 h) > 1,000 mg/l Test performed using a similar product. (OECD Test Guideline 209)

Ecotoxicology Assessment

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- Acute aquatic toxicity : Toxic to aquatic life.
- Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

**Persistence and degradability**

- Biodegradability : Readily biodegradable.  
76 % (28 d)  
(OECD Test Guideline 301F)  
Test performed using a similar product.

**Bioaccumulative potential**

- Bioaccumulation : Bioconcentration factor (BCF): 586  
Method: calculated value  
The product may be accumulated in organisms.
- Partition coefficient: n-octanol/water : log Pow ca. 4.5 - 5.0 ( 25 °C ; OECD Test Guideline 117)  
Test performed using a similar product.

**Mobility in soil**

- Distribution among environmental compartments : Adsorption/Soil  
log Koc 3.0 (calculated value)

**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 : Discharge into the environment must be avoided.  
Do not contaminate ponds, waterways or ditches with chemical 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.



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

UN/ID No. : UN 3082  
Proper shipping name : Environmentally hazardous substance, liquid, n.o.s.  
(3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one,  
3-methyl-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.  
(3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one,  
3-methyl-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.  
(3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one,  
3-methyl-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 (3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one  
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one )  
Remarks : No additional requirements.

**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** : Acute Health Hazard

**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 I 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**

3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5	90 - 100 %
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-89-0	5 - 10 %
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	7779-30-8	5 - 10 %

**New Jersey Right To Know**

3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5	90 - 100 %
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-89-0	5 - 10 %
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	7779-30-8	5 - 10 %

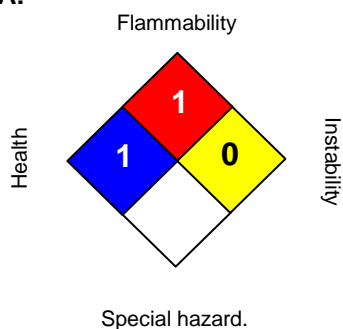
**The components of this product are reported in the following inventories:**

**TSCA** : On TSCA Inventory

## SECTION 16. OTHER INFORMATION

## Further information

## NFPA:



## HMIS III:

<b>HEALTH</b>	<b>2</b>
<b>FLAMMABILITY</b>	<b>1</b>
<b>PHYSICAL HAZARD</b>	<b>0</b>

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.