

SECTION 1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Isonaline 70
Substance name : Ionone, methyl-
CAS-No. : 1335-46-2

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 Responsible/issuing person : sds.nutritionalproducts@dsm.com

1.4 Emergency telephone number

+41 62 866 2314

SECTION 2. HAZARDS IDENTIFICATION**Emergency Overview**

CAUTION	
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

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

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.

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

Synonyms : Methyl ionone

Brief description of the product : Multi constituent substance
Mixture of isomers

Molecular formula : C₁₄H₂₂O

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	50 - 70
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	7779-30-8	20 - 30
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-89-0	10 - 20
1-(2,6,6-trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one	127-43-5	5 - 10

SECTION 4. FIRST AID MEASURES

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

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	: 259 °F (126 °C) at 1,013 hPa (101,300 mm/HG) Method: ISO 2719
Ignition temperature	: 254 °C (at 1,013 hPa)
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	: Dry chemical Alcohol-resistant foam
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

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

- 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 : Keep under inert gas.
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.
Hazardous components without workplace control parameters

Personal protective equipment

- Respiratory protection : In the case of vapour formation use a respirator with an approved filter.
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
Melting point/range	: < -20 °C
Boiling point/boiling range	: 270.6 °C (at 1,013 hPa)
Flash point	: 126 °C (1,013 hPa, closed cup, ISO 2719)
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	: 0.0022 hPa (at 20 °C)
Relative vapour density	: not determined
Density	: 0.93 g/cm ³ (at 20 °C)
Water solubility	: 21 - 44 mg/l (20 °C)
Solubility in other solvents	: various organic solvents: soluble
Partition coefficient: n-octanol/water	: log Pow 4.5 - 5.0 (23 °C)
Ignition temperature	: 254 °C (at 1,013 hPa)
Thermal decomposition	: Not relevant
Viscosity, dynamic	: 13.1 mPa.s (at 20 °C)
Explosive properties	: Not explosive

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

Oxidizing properties : Not oxidizing

9.2 Other information

Refractive index : 1.498 - 1.502 (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 : 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, male and female): > 5,000 mg/kg

Skin irritation : Moderate skin irritation (Rabbit)

Eye irritation : Irritating to eyes. (Rabbit)

Sensitisation : Did not cause sensitization. (Guinea pig, Maximisation Test (GPMT))
: no photoallergenic skin reaction (Guinea pig)

Carcinogenicity : No indication for carcinogenicity known.

Genotoxicity in vitro : not mutagenic (Ames test)

Genotoxicity in vivo : not genotoxic (In vivo micronucleus test, Mouse)

Reproductive toxicity : No indication for adverse effects on fertility known.

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

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 (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	: Daphnia magna (Water flea) EC50 (48 h) 3.7 mg/l (OECD Test Guideline 202)
Toxicity to algae	: Desmodesmus subspicatus (green algae) EC50 (72 h) > 9.42 mg/l (OECD Test Guideline 201)
Toxicity to bacteria	: activated sludge EC50 (1 h) > 1,000 mg/l (OECD Test Guideline 209)

Persistence and degradability

Biodegradability	: Readily biodegradable 76 % (28 d) (OECD Test Guideline 301F)
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Bioaccumulative potential

Bioaccumulation	: Bioconcentration factor (BCF): 586 Method: calculated value
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SAFETY DATA SHEET

**Isonaline 70****5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

The product may be accumulated in organisms.

Partition coefficient: n-octanol/water : log Pow 4.5 - 5.0 (23 °C)

Mobility in soil

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

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

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.

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,
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one)
Class : 9
Packing group : III
Labels : Miscellaneous Dangerous Goods
Packing instruction (cargo) : 964

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

aircraft)

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, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-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 substance, liquid, n.o.s.
(3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-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, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one)

Special precautions for user

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.

Isonaline 70**5005817**

Version 3.1

Revision Date 11/23/2015

Print Date 03/02/2018

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

3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5	70 - 90 %
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	7779-30-8	30 - 50 %
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-89-0	10 - 20 %
1-(2,6,6-trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one	127-43-5	10 - 20 %

New Jersey Right To Know

3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5	70 - 90 %
1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	7779-30-8	30 - 50 %
3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-89-0	10 - 20 %
1-(2,6,6-trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one	127-43-5	10 - 20 %

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

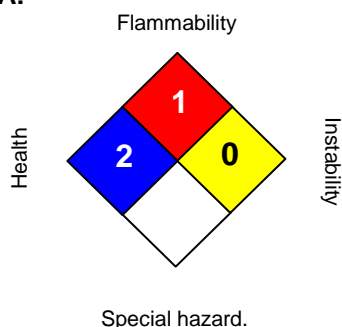
TSCA

: On TSCA Inventory

SECTION 16. OTHER INFORMATION

Further information

NFPA:



HMIS III:

HEALTH	3
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.