

Safety Data Sheet
according to Regulation (EC) No. 1907/2006 (REACH)



Trade name : PFW® DIHYDRO ISOJASMONATE
Revision date : 10.06.2014
Print date : 26-05-2015

Version (Revision) : 2.0.3 (2.0.2)

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

1.1 Product identifier

PFW® DIHYDRO ISOJASMONATE (W00341)
methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5 ; EC No. : 253-379-1

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

Relevant identified uses

Fragrance ingredient which may be used in fragrance compounds according to the current legislation and IFRA rules.
Reserved for industrial and professional use.

Uses advised against

Not intended for oral consumption.

1.3 Details of the supplier of the safety data sheet

Supplier (manufacturer/importer/only representative/downstream user/distributor)

PFW Aroma Chemicals B.V.

Street : Veemweg 29-31

Postal code/city : NL - 3371 MT Barneveld

Telephone : +31 342 40 77 00

Telefax : +31 342 40 77 20

Information contact : pfw@pfw.nl

1.4 Emergency telephone number

+31 342 40 77 93

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

None

Hazard classes and hazard categories

Skin Irrit. 3

Classification according to Directive 67/548/EEC or 1999/45/EC

None

2.2 Label elements

None

2.3 Other hazards

None

SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name : methyl 2-hexyl-3-oxocyclopentanecarboxylate

EC No. : 253-379-1

CAS No. : 37172-53-5

Purity : ≥ 98 % [mass]

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Synonymes

INCI : METHYL HEXYL CYCLOPENTANONE CARBOXYLATE

SECTION 4: First aid measures

4.1 Description of first aid measures

General information

When in doubt or if symptoms are observed, get medical advice. Remove victim out of the danger area. Put victim at rest, cover with a blanket and keep warm. Do not leave affected person unattended. If unconscious place in recovery position and seek medical advice.

In case of inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

In case of skin contact

Wash immediately with: Water Do not wash with: Solvents/Thinner

After eye contact

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

Rinse mouth immediately and drink plenty of water. Let water be drunken in little sips (dilution effect). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

No information available.

4.3 Indication of any immediate medical attention and special treatment needed

None

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

alcohol resistant foam. Extinguishing powder.

Unsuitable extinguishing media

Strong water jet. Water mist.

5.2 Special hazards arising from the substance or mixture

Hazardous combustion products

In case of fire may be liberated: Carbon dioxide (CO₂) Carbon monoxide (CO).

5.3 Advice for firefighters

Do not inhale explosion and combustion gases. Use water spray jet to protect personnel and to cool endangered containers.

Special protective equipment for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Special danger of slipping by leaking/spilling product. See protective measures under point 7 and 8.

6.2 Environmental precautions

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In case of entry into waterways, soil or drains, inform the responsible authorities.

6.3 Methods and material for containment and cleaning up

Suitable material for taking up: Sand, Kieselguhr, Universal binder, Sawdust. Collect in closed and suitable containers for disposal.

6.4 Reference to other sections

See protective measures under point 7 and 8.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work. Wear personal protection equipment (see chapter 8).

7.2 Conditions for safe storage, including any incompatibilities

Technical measures and storage conditions

Keep the packing dry and well sealed to prevent contamination and absorption of humidity. Never use pressure to empty container.

Hints on joint storage

Keep away from oxidising agent, acid and alkali.

Storage class : 10

Storage class (TRGS 510) : 10

7.3 Specific end use(s)

None

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

To date, no national critical limit values exist.

8.2 Exposure controls

When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work.

Appropriate engineering controls

No special technical protective measures are necessary.

Personal protection equipment

Eye/face protection

Eye glasses with side protection

Skin protection

Hand protection

Hand protection is not required

Body protection

Overall

Respiratory protection

Respiratory protection necessary at: exceeding exposure limit values insufficient ventilation insufficient exhaust Handling larger quantities. Container device with compressed air (DIN EN 137) / Filtering device (full mask or mouthpiece) with filter: Filter types: A, B, E, K. Class 1: Maximum permitted contaminant concentration in inhaled air = 1000 mL/m³ (0.1 % by vol.); class 2: maximum permitted contaminant concentration in inhaled air = 5000 mL/m³ (0.5 % by vol.); class 3: maximum permitted contaminant concentration in inhaled air = 10000 mL/m³ (1.0 % by vol.)

Environmental exposure controls

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Send to a hazardous waste incinerator facility under observation of official regulations.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Safety relevant basis data

Physical state :			liquid	
Colour :			colourless to pale yellow	
Odour :			floral	
Boiling temperature/boiling range :	(1013 hPa)	ca.	309 °C	
Decomposition temperature :	(1013 hPa)		No data available	
Freezing point :		<	-20 °C	
Flash point (Closed Cup) :		>	100 °C	DIN EN 51578
Auto-ignition temperature :			No data available	
Lower explosion limit :			No data available	
Upper explosion limit :			No data available	
Explosive properties :			none	
Vapour pressure :	(50 °C)	ca.	0,01 hPa	
Vapour pressure :	(20 °C)	<	0,01 hPa	
Evaporation rate (n-butylacetate = 1) :			No data available	
Relative density (water = 1) :	(20 °C)	ca.	0,993	
Density :	(20 °C)		0,995 g/cm ³	
Water solubility :	(20 °C)		0,186 g/l	
pH value :			No data available	
Log Pow :			3,2	
Viscosity :	(20 °C)		No data available	NEN-ISO 2884
Odour threshold :			No data available	
Vapour density (air = 1) :	(1013 hPa / 20 °C)		1	
Oxidising properties :			none	

9.2 Other information

None

SECTION 10: Stability and reactivity

10.1 Reactivity

No information available.

10.2 Chemical stability

No information available.

10.3 Possibility of hazardous reactions

No information available.

10.4 Conditions to avoid

No information available.

10.5 Incompatible materials

Exothermic reaction with: oxidising agent strong acid strong alkali

10.6 Hazardous decomposition products

Decomposition with: Carbon dioxide (CO₂). Carbon monoxide (CO).

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute effects

Acute oral toxicity

Parameter : LD50 (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Exposure route : Oral
Species : Rat
Effective dose : > 5000 mg/kg

Acute dermal toxicity

Parameter : LD50 (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Exposure route : Dermal
Species : Rabbit
Effective dose : > 5000 mg/kg

SECTION 12: Ecological information

12.1 Toxicity

Aquatic toxicity

No information available.

Acute (short-term) fish toxicity

Parameter : LC50 (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Species : Acute (short-term) fish toxicity
Effective dose : 10 - 100 mg/l
Exposure time : 96 h
Methode : QSAR
Source : PFW Aroma Chemicals BV

Acute (short-term) daphnia toxicity

Parameter : EC50 (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Species : Acute (short-term) daphnia toxicity
Effective dose : 10 - 100 mg/l
Exposure time : 48 h
Methode : QSAR
Source : PFW Aroma Chemicals BV

Acute (short-term) algae toxicity

Parameter : EC50 (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Species : Algal inhibition
Effective dose : 12 mg/l
Exposure time : 72 h
Methode : OECD 201
Source : PFW Aroma Chemicals BV

12.2 Persistence and degradability

Biodegradation

Analytical method : Biodegradation (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Parameter : Degree of elimination
Type : Aerobic
Degradation rate : 73,1 %
Time : 28 days
Methode : Biological Oxygen Demand test for Insoluble Substances (ISO/DIS method 10708)
Source : PFW Aroma Chemicals BV

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12.3 Bioaccumulative potential

Parameter : Bioconcentration factor (BCF) (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Species : Bioconcentration factor (BCF)
Result : ca. 43 l/kg ww
Methode : QSAR
Source : PFW Aroma Chemicals BV
Parameter : Partition coefficient n-octanol /water (log P O/W) (methyl 2-hexyl-3-oxocyclopentanecarboxylate ; CAS No. : 37172-53-5)
Species : Partition coefficient n-octanol /water (log P O/W)
Result : 3,2
Source : PFW Aroma Chemicals BV

Based on the n-octanol/water partition coefficient accumulation in organisms is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6 Other adverse effects

None

12.7 Further ecological information

None

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Send to a hazardous waste incinerator facility under observation of official regulations. Clean IBCs or drums at approved facility only. Contaminated packages must be completely emptied and can be re-used following proper cleaning. Packing which cannot be properly cleaned must be disposed of. Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information

14.1 UN number

No dangerous goods in sense of this transport regulation.

14.2 UN proper shipping name

No dangerous goods in sense of this transport regulation.

14.3 Transport hazard class(es)

No dangerous goods in sense of this transport regulation.

14.4 Packing group

No dangerous goods in sense of this transport regulation.

14.5 Environmental hazards

No dangerous goods in sense of this transport regulation.

14.6 Special precautions for user

None

SECTION 15: Regulatory information

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

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mixture

National regulations

Water hazard class (WGK)

Class : slightly water pollutant according VwVwS

Other regulations, restrictions and prohibition regulations

TSCA (USA) : listed

CEPA (Canada) : NDSL

India : not applicable

ENCS (Japan) : 3 - 4578

ISHL (Japan) : not listed

IECSC (China) : listed

ECL (Korea) : not listed

PICCS (Philippines) : listed

AICS (Australia) : listed

NZIoC (New Zealand) : group standard

15.2 Chemical Safety Assessment

Chemical safety assessments for substances in this mixture were not carried out.

SECTION 16: Other information

16.1 Indication of changes

None

16.2 Abbreviations and acronyms

a.i. = Active ingredient; ACGIH = American Conference of Governmental Industrial Hygienists (US); ADR = European Agreement concerning the International Carriage of Dangerous Goods by Road; AFFF = Aqueous Film Forming Foam; AICS = Australian Inventory of Chemical Substances; AISE = International Association for Soaps, Detergents and Maintenance Products (joint project of AISE and CEFIC); AOAC = AOAC International (formerly Association of Official Analytical Chemists); aq. = Aqueous; Asia-PAC = Asia Pacific; ASTM = American Society of Testing and Materials (US); atm = Atmosphere(s); B.V. = Beperkt Vennootschap (LTD = Limited); BCF = Bioconcentration Factor; bp = Boiling point at stated pressure; bw = Body weight; ca = (Circa) about; CAS No = Chemical Abstracts Service Number (see ACS - American Chemical Society); CEFIC = European Chemical Industry Council (established 1972); CEPA = Canadian Environmental Protection Act (CAN); CEPA = Canadian Environmental Protection Act (Canada); CIPAC = Collaborative International Pesticides Analytical Council; CLP = REGULATION (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.; CoE = Council of Europe (EU); Conc = Concentration; cP = CentiPoise; CSNN = Chemical Substance Nomination & Notification (Taiwan); cSt = Centistokes; d = Day(s); DIN = Deutsches Institut für Normung e.V.; DNEL = Derived No-Effect Level; DSL = Domestic Substances List; DT50 = Time for 50% loss; half-life; EbC50 = Median effective concentration (biomass, e.g. of algae); EC = European Community; European Commission; EC50 = Median effective concentration; ECL = Existing Chemicals List (Korea); EINECS = European Inventory of Existing Commercial Chemical Substances (EU, outdated, now replaced by EC Number); ELINCS = European List of Notified (New) Chemicals; ENCS = Existing and New Chemical Substances Inventory (Japan); ErC50 = Median effective concentration (growth rate, e.g. of algae); EU = European Union; EWC = European Waste Catalogue; FAO = Food and Agriculture Organization (United Nations); FEMA = Flavor & Extract Manufacturers Association (USA); FLAVIS = Flavour Information System (EU); GIFAP = Groupement International des Associations Nationales de Fabricants de Produits Agrochimiques (now CropLife International); GRAS = Generally Recognized As Safe (USA); h = Hour(s); hPa = HectoPascal (unit of pressure); IARC = International Agency for Research on Cancer; IATA = International Air Transport Association; IC50 = Concentration that produces 50% inhibition; IECSC = Inventory of Existing Chemical Substances (China); IMDG Code = International Maritime Dangerous Goods Code; IMO = International Maritime Organization; ISO = International Organization for Standardization; IUCLID = International Uniform Chemical Information Database; IUPAC = International Union of Pure and Applied Chemistry; IVIS = In-Vitro Irritancy Score; JECFA = Joint Expert Committee on Food Additives (United Nations); kg = Kilogram; Kow = Distribution coefficient between n-octanol and water; kPa = KiloPascal (unit of pressure); LC50 = Concentration required to kill 50% of test organisms; LD50 = Dose required to kill 50% of test organisms; LEL = Lower Explosive Limit/Lower Explosion Limit; LOAEL = Lowest observed

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adverse effect level; LVE = Low Volume Exemption; mg = Milligram; min = Minute(s); ml = Milliliter; mmHg = Pressure equivalent to 1 mm of mercury (133.3 Pa); mp = Melting point; MRL = Maximum Residue Limit; MSDS = Material Safety Data Sheet; n.o.s. = Not Otherwise Specified; NDSL = Non-Domestic Substances List; NIOSH = National Institute for Occupational Safety and Health (US); NOAEL = No Observed Adverse Effect Level; NOEC = No observed effect concentration; NOEL = No Observable Effect Level; NOx = Oxides of Nitrogen; NZIoC = New Zealand Inventory of Chemicals; OECD = Organization for Economic Cooperation and Development; OEL = Occupational Exposure Limits; Pa = Pascal (unit of pressure); PBT = Persistent, Bioaccumulative or Toxic; pH = -log₁₀ hydrogen ion concentration; PICCS = Philippine Inventory of Chemicals and Chemical Substances; pKa = -log₁₀ acid dissociation constant; PNEC = Predicted No Effect Concentration; POPs = Persistent Organic Pollutants; ppb = Parts per billion; PPE = Personal Protection Equipment; ppm = Parts per million; ppt = Parts per trillion; PVC = Polyvinyl Chloride; QSAR = Quantitative Structure-Activity Relationship; REACH = Registration, Evaluation and Authorization of Chemicals (EU, see NCP); SI = International System of Units; STEL = Short-Term Exposure Limit; tech. = Technical grade; TSCA = Toxic Substances Control Act (US); TSCA = Toxic Substances Control Act (USA); TWA = Time-Weighted Average; UN = United Nations; vPvB = Very Persistent and Very Bioaccumulative; VwVwS = Verwaltungsvorschrift wassergefährdender Stoffe; WHO = World Health Organization = OMS; y = Year(s);

16.3 Key literature references and sources for data

None

16.4 Relevant R-, H- and EUH-phrases (Number and full text)

None

16.5 Training advice

None

16.6 Additional information

None

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.