

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



**Trade name :** METHYL OCTALACTONE  
**Revision date :** 30.04.2014  
**Print date :** 27-05-2015

**Version (Revision) :** 1.0.3 (1.0.2)

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

**1.1 Product identifier**

METHYL OCTALACTONE (W00757)  
5-butylidihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 ; EC No. : 254-357-4

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

**Relevant identified uses**

Flavour and fragrance ingredient. 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**

-

**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**

None

**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 :** 5-butylidihydro-4-methylfuran-2(3H)-one

**EC No. :** 254-357-4

**CAS No. :** 39212-23-2

**Purity :** ≥ 98 % [mass]

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## Synonymes

IUPAC : 5-butyl-4-methyldihydrofuran-2(3H)-one

INCI : 3-METHYL-GAMMA-OCTALACTONE

## 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 (CO<sub>2</sub>) 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.

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## 6.2 Environmental precautions

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/m<sup>3</sup> (0.1 % by vol.); class 2: maximum permitted contaminant concentration in inhaled air = 5000 mL/m<sup>3</sup> (0.5 % by vol.); class 3: maximum permitted contaminant concentration in inhaled air = 10000 mL/m<sup>3</sup> (1.0 % by vol.)

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## Environmental exposure controls

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

**Odour threshold in air :** No data available

#### Safety relevant basis data

<b>Physical state :</b>			liquid	
<b>Colour :</b>			colourless to pale yellow	
<b>Odour :</b>			intense sweet	
<b>Boiling temperature/boiling range :</b>	( 1013 hPa )	ca.	260 °C	
<b>Freezing point :</b>		<	-20 °C	
<b>Flash point (Closed Cup) :</b>		>	100 °C	DIN EN 51578
<b>Auto-ignition temperature :</b>			No data available	
<b>Lower explosion limit :</b>			No data available	
<b>Upper explosion limit :</b>			No data available	
<b>Explosive properties :</b>			none	
<b>Vapour pressure :</b>	( 50 °C )	ca.	0,17 hPa	
<b>Evaporation rate (n-butylacetate = 1) :</b>			No data available	
<b>Surface tension (20°C) :</b>	( 20 °C )		No data available	
<b>Relative density (water = 1) :</b>	( 20 °C )		0,957 - 0,965	
<b>Density :</b>	( 20 °C )		0,959 - 0,967 g/cm <sup>3</sup>	
<b>pH value :</b>			No data available	
<b>Log Pow :</b>		ca.	3	
<b>Viscosity :</b>	( 20 °C )		No data available	NEN-ISO 2884
<b>Vapour density (air = 1) :</b>	( 1013 hPa / 20 °C )		1	
<b>Oxidising properties :</b>			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 (CO<sub>2</sub>). Carbon monoxide (CO).

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute effects

##### Acute oral toxicity

Parameter : LD50 ( 5-butyldihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Exposure route : Oral  
Species : Rat  
Effective dose : > 9660 mg/kg  
Methode : OECD 401 Acute Oral Toxicity  
Source : PFW Aroma Chemicals BV

#### Irritant and corrosive effects

##### Primary irritation to the skin

Parameter : Irritation of the skin ( 5-butyldihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : Albino rabbit  
Parameter : in-vivo  
Result : No Irritation  
Methode : OECD 404 Acute Dermal Irritation/Corrosion  
Source : PFW Aroma Chemicals BV

#### Sensitisation

##### In case of skin contact

Parameter : Skin sensitisation ( 5-butyldihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : Guinea pig  
Parameter : in-vivo  
Result : not sensitising  
Methode : OECD 406 Skin Sensitisation  
Source : PFW Aroma Chemicals BV  
Parameter : Skin sensitisation ( 5-butyldihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : Guinea pig  
Parameter : in-vivo  
Result : no photosensitisation  
Methode : Draize  
Source : PFW Aroma Chemicals BV  
Parameter : Skin sensitisation ( 5-butyldihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : rabbit  
Parameter : in-vivo  
Result : not phototoxic  
Methode : Draize  
Source : PFW Aroma Chemicals BV

## SECTION 12: Ecological information

### 12.1 Toxicity

#### Aquatic toxicity

No information available.

#### Acute (short-term) fish toxicity

Parameter : LC50 ( 5-butyldihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : Acute (short-term) fish toxicity  
Effective dose : 10 - 100 mg/l

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Exposure time : 96 h  
Methode : QSAR  
Source : PFW Aroma Chemicals BV

#### Acute (short-term) daphnia toxicity

Parameter : EC50 ( 5-butylidihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
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 ( 5-butylidihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : Acute (short-term) algae toxicity  
Effective dose : 10 - 100 mg/l  
Exposure time : 96 h  
Methode : QSAR  
Source : PFW Aroma Chemicals BV

## 12.2 Persistence and degradability

### Biodegradation

Analytical method : Biodegradation ( 5-butylidihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Parameter : Degree of elimination  
Type : Aerobic  
Degradation rate : 98 %  
Time : 28 days  
Evaluation : readily biodegradable (>73% degraded after 28 days)  
Methode : Closed Bottle Test (Method OECD 301D)  
Source : PFW Aroma Chemical BV

## 12.3 Bioaccumulative potential

Parameter : Bioconcentration factor (BCF) ( 5-butylidihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Species : BCF  
Result : ca. 10 l/kg ww  
Methode : QSAR  
Source : PFW Aroma Chemicals BV  
Parameter : Partition coefficient n-octanol/water (log P O/W) ( 5-butylidihydro-4-methylfuran-2(3H)-one ; CAS No. : 39212-23-2 )  
Result : ca. 2  
Methode : QSAR  
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

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### 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 mixture

#### National regulations

##### Water hazard class (WGK)

Class : water pollutant according VwVwS

##### Other regulations, restrictions and prohibition regulations

TSCA (USA) : listed

CEPA (Canada) : DSL

India : not applicable

ENCS (Japan) : not listed

ISHL (Japan) : not listed

IECSC (China) : listed

ECL (Korea) : not listed

PICCS (Philippines) : listed

AICS (Australia) : listed

NZIoC (New Zealand) : group standard

FLAVIS (EU) : listed FL 10 - 53

CoE (EU) : listed 10 - 535

JECFA (UN) : listed 437

FEMA (USA) : listed 3803

GRAS (USA) : listed 17

### 15.2 Chemical Safety Assessment

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

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### 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 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 = -log<sub>10</sub> hydrogen ion concentration; PICCS = Philippine Inventory of Chemicals and Chemical Substances; pKa = -log<sub>10</sub> 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



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None

## 16.6 Additional information

None

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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.

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