

Safety Data Sheet

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



Trade name : KEFLOROL 90
Revision date : 19.08.2015
Print date : 19-8-2015

Version : 1.0.0

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

1.1 Product identifier

KEFLOROL 90 (C60093)

2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; REACH registration No. : 01-0000015458-64-0010 ; CAS No. : 63500-71-0 ; EC No. : 405-040-6 ; INDEX No. : 603-101-00-3

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]

Eye Irrit. 2 ; H319 - Serious eye damage/eye irritation : Category 2A ; Causes serious eye irritation.

Hazard classes and hazard categories

Eye Irrit. 2

Eye Irrit. 2

2.2 Label elements

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

Hazard pictograms



Exclamation mark (GHS07)

Signal word

Warning

Hazard statements

H319 Causes serious eye irritation.

Precautionary statements

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P264	Wash hands thoroughly after handling.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P337+P313	If eye irritation persists: Get medical advice/attention.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3 Other hazards

None

SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name : 2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans)

INDEX No. : 603-101-00-3

EC No. : 405-040-6

REACH No. : 01-0000015458-64-0010

CAS No. : 63500-71-0

Purity : ≥ 98 % [mass]

Synonymes

IUPAC : Tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyran-4-ol

INCI : TETRAHYDRO-METHYL-METHYLPROPYL)-PYRAN-4-OL

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. Call a physician immediately.

After ingestion

If accidentally swallowed rinse the mouth with plenty of water (only if the person is conscious) and obtain immediate medical attention. Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

Irritating to eyes.

4.3 Indication of any immediate medical attention and special treatment needed

None

SECTION 5: Firefighting measures

5.1 Extinguishing media

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

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. Do not breathe gas/fumes/vapour/spray. Provide adequate ventilation. Remove persons to safety. See protective measures under point 7 and 8.

6.2 Environmental precautions

Ensure all waste water is collected and treated via a waste water treatment plant. 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

Provide adequate ventilation as well as local exhaust at critical locations. When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work. All work processes must always be designed so that the following is as low as possible: eye contact, skin contact. In case of entry into waterways, soil or drains, inform the responsible authorities. 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

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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

Gloves. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. Breakthrough times and swelling properties of the material must be taken into consideration.

Suitable material : Butyl caoutchouc (butyl rubber)

Breakthrough time (maximum wearing time) : >480 min.

Thickness of the glove material : 1.00 mm.

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

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 :			fresh clean soft natural floral muguet	
Boiling temperature/boiling range :	(1013 hPa)		229,6	°C
Decomposition temperature :	(1013 hPa)		No data available	
Freezing point :		<	-20	°C
Flash point (Closed Cup) :		>	100	°C
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.	0,35	hPa
Vapour pressure :	(20 °C)		0,013	hPa
Evaporation rate (n-butylacetate =			No data available	

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1) :				
Surface tension (20°C)	(20 °C)	ca.	52	mN/m
Relative density (water = 1) :	(20 °C)		0,95	
Density :	(25 °C)		0,944 - 0,954	g/cm ³
Solubility in water :	(25 °C)	ca.	25	g/l
pH value :			No data available	
Log Pow :			2,2	
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).

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Irritating to eyes.

Acute effects

Acute oral toxicity

Parameter :	LD50 (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Exposure route :	Oral
Species :	Rat
Effective dose :	> 5000 mg/kg
Exposure time :	14 days
Methode :	OECD 401 Acute Oral Toxicity
Source :	Kelkar Aroma Chemicals Division

Acute dermal toxicity

Parameter :	LD50 (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Exposure route :	Dermal
Species :	Rabbit
Effective dose :	> 2000 mg/kg
Methode :	OECD 402
Source :	Kelkar Aroma Chemicals Division

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Irritant and corrosive effects

Primary irritation to the skin

Parameter : Irritation of the skin (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Species : Guinea pig
Result : No irritation
Methode : OECD 404 Acute Dermal Irritation/Corrosion
Source : Kelkar Aroma Chemicals Division

Irritation to eyes

Parameter : Irritation of the eyes (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Species : Albino rabbit
Result : Corneal opacity. Conjunctival redness.
Methode : OECD 405 Acute eye irritation/corrosion
Source : Kelkar Aroma Chemicals Division

Sensitisation

In case of skin contact

Parameter : Skin sensitisation (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Parameter : guinea pig
Result : not sensitising
Methode : OECD 406 Skin Sensitisation
Source : Kelkar Aroma Chemicals Division

Repeated dose toxicity (subacute, subchronic, chronic)

Subacute oral toxicity

Parameter : NOAEL(C) (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Exposure route : Oral
Species : rat
Effective dose : 125 mg/kg bw/day
Methode : OECD 407 Repeated Dose 28-day Oral Toxicity Study in Rodents
Source : Kelkar Aroma Chemicals Division

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)

Germ cell mutagenicity/Genotoxicity

In vitro mutagenicity

Parameter : Gene-mutations microorganisms (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Exposure route : In vitro mutagenicity
Species : Escherichia coli
Test result : Negative (with metabolic activation). Negative (without metabolic activation).
Methode : OECD 471: Ames test
Source : Kelkar Aroma Chemicals Division

Parameter : Gene-mutations microorganisms (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Exposure route : In vitro mutagenicity
Species : Salmonella typhimurium
Test result : Negative (with metabolic activation). Negative (without metabolic activation).
Methode : OECD 471: Ames test
Source : Kelkar Aroma Chemicals Division

Parameter : Chromosomal aberrations mammalian cells (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Exposure route : In vitro mutagenicity

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Species : Human lymphocytes
Test result : Negative (with metabolic activation). Negative (without metabolic activation).
Methode : OECD 473 in vitro mammalian chromosome aberration test
Source : Kelkar Aroma Chemicals Division

SECTION 12: Ecological information

12.1 Toxicity

Aquatic toxicity

Acute (short-term) fish toxicity

Parameter : LC50 (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Species : Oncorhynchus mykiss (Rainbow trout)
Evaluation parameter : Acute (short-term) fish toxicity
Effective dose : 354 mg/l
Exposure time : 96 h
Methode : OECD 203 Acute toxicity for fish
Source : Kelkar Aroma Chemicals Division

Acute (short-term) daphnia toxicity

Parameter : EC50 (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Species : Daphnia magna (Big water flea)
Evaluation parameter : Acute (short-term) daphnia toxicity
Effective dose : 803 mg/l
Exposure time : 48 h
Methode : OECD 202 Daphnia sp. Acute immobilisation test
Source : Kelkar Aroma Chemicals Division

Acute (short-term) algae toxicity

Parameter : EC50 (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Species : Scenedesmus subspicatus
Evaluation parameter : Acute (short-term) algae toxicity
Effective dose : 94 mg/l
Exposure time : 72 h
Methode : OECD 201 Freshwater algae and cyanobacteria, growth inhibition test
Source : Kelkar Aroma Chemicals Division

Effects in sewage plants

Parameter : EC50 (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Inoculum : Municipal
Evaluation parameter : Effects in sewage plants
Effective dose : > 1000 mg/l
Methode : OECD 209
Source : Kelkar Aroma Chemicals Division

12.2 Persistence and degradability

Biodegradation

Analytical method : Biodegradation (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)
Type : Aerobic
Evaluation : Not readily biodegradable (according to OECD criteria)
Methode : Modified MITI test

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Source : Kelkar Aroma Chemicals Division

12.3 Bioaccumulative potential

Parameter : Partition coefficient n-octanol/water (log P O/W) (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)

Result : 1,65

Methode : OECD 107 Shake Flask Method

Source : Kelkar Aroma Chemicals Division

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

12.4 Mobility in soil

Adsorption/Desorption

Parameter : Adsorption coefficient (2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2-methylpropyl)- mixed isomers (cis and trans) ; CAS No. : 63500-71-0)

Log Koc : 1,4

Methode : OECD 121

Source : Kelkar Aroma Chemicals Division

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

No information available.

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

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

National regulations

Water hazard class (WGK)

Class : slightly water pollutant according VwVwS

Other regulations, restrictions and prohibition regulations

TSCA (USA) : listed

CEPA (Canada) : DSL

Asia-PAC : listed

India : not applicable

ENCS (Japan) : not listed

ISHL (Japan) : listed 8- 4 - 1494

IECSC (China) : listed

CSNN (Taiwan) : listed

ECL (Korea) : listed 2005 - 33059

PICCS (Philippines) : listed

AICS (Australia) : listed

NZIoC (New Zealand) : listed

FLAVIS (EU) : not listed

CoE (EU) : not listed

JECFA (UN) : not listed

FEMA (USA) : not listed

GRAS (USA) : not listed

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

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Agrochimiques (now CroLife 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 = -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)

H319 Causes serious eye irritation.
36 Irritating to eyes.

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.