

Acetylacetone for synthesis

Revision date: 27.05.2022

Product code: 19626

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

1.1. Product identifier

Acetylacetone for synthesis

Substance name: pentane-2,4-dione; acetylacetone
REACH Registration Number: 01-2119458968-15-XXXX
CAS No: 123-54-6
Index No: 606-029-00-0
EC No: 204-634-0

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

Use of the substance/mixture

Laboratory chemical
Industrial uses: Uses of substances as such or in preparations at industrial sites
Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: Fa. Bernd Kraft GmbH
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
Telefax: 0203/5194-290
e-mail: info@berndkraft.de
Contact person: Abteilung Produktsicherheit
Telephone: 0203/5194-107/117
e-mail: produktsicherheit@berndkraft.de
Internet: www.berndkraft.de
Responsible Department: Abteilung Produktsicherheit

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

No data available

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 3; H226
Acute Tox. 3; H331
Acute Tox. 3; H311
Acute Tox. 4; H302

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Hazard components for labelling

pentane-2,4-dione

Signal word: Danger

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Pictograms:



Hazard statements

H226 Flammable liquid and vapour.
H302 Harmful if swallowed.
H311+H331 Toxic in contact with skin or if inhaled.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P241 Use explosion-proof electrical/ventilating/lighting equipment.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₅H₈O₂
Molecular weight: 100,12 g/mol

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
123-54-6	pentane-2,4-dione			100 %
	204-634-0	606-029-00-0	01-2119458968-15-	
	Flam. Liq. 3, Acute Tox. 3, Acute Tox. 3, Acute Tox. 4; H226 H331 H311 H302			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
123-54-6	204-634-0	pentane-2,4-dione	100 %
		inhalation: LC50 = 1224 mg/l (vapours); inhalation: ATE = 0,5 mg/l (dusts or mists); dermal: LD50 = 790 mg/kg; oral: LD50 = 760 mg/kg	

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

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General information

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down.

After inhalation

Provide fresh air.

Call a physician immediately.

After contact with skin

Wash immediately with: Water

Take off immediately all contaminated clothing and wash it before reuse.

Call a physician immediately.

After contact with eyes

After eye contact: Rinse immediately carefully and thoroughly with eye-bath or water. Consult an ophthalmologist.

After ingestion

Call a physician immediately. Observe risk of aspiration if vomiting occurs.

4.2. Most important symptoms and effects, both acute and delayed

irritant.

Cough

Dyspnoea

Respiratory complaints

Dizziness

Unconsciousness

Vomiting

Headache

4.3. Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Water spray jet, Carbon dioxide (CO₂), Foam, Extinguishing powder.

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquids

Hazardous combustion products Vapours are heavier than air, spread along floors and form explosive mixtures with air.

5.3. Advice for firefighters

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

Additional information

Danger of bursting container.

Use water spray jet to protect personnel and to cool endangered containers.

Suppress gases/vapours/mists with water spray jet.

Move undamaged containers from immediate hazard area if it can be done safely.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

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This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).

Take action to prevent static discharges.

For non-emergency personnel

Provide adequate ventilation.

Use personal protection equipment.

Avoid contact with skin, eyes and clothes.

Remove persons to safety.

Emergency procedures

Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.

Danger of explosion

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.

Prevent spread over a wide area (e.g. by containment or oil barriers).

Collect in closed and suitable containers for disposal.

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.

Do not breathe dust/fume/gas/mist/vapours/spray.

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Read label before use. Handle and open container with care.

When using do not eat, drink, smoke, sniff. Keep container tightly closed.

Use personal protection equipment. Use extractor hood (laboratory).

Do not breathe gas/fumes/vapour/spray. Provide adequate ventilation.

Draw up and observe skin protection programme.

Wash hands and face before breaks and after work and take a shower if necessary.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

Vapours can form explosive mixtures with air.

Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

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Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.
If handled uncovered, arrangements with local exhaust ventilation have to be used.
Store in a place accessible by authorized persons only.
storage temperature : 15°C - 25°C

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaust at critical locations. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Hints on joint storage

Do not store together with: Oxidising agent. Pyrophoric or self-heating substances.

Further information on storage conditions

Keep cool. Protect from sunlight.

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Occupational exposure limits

CAS No	Substance	ppm	mg/m ³	fib/cm ³	Category	Origin
123-54-6	2,4-Pentanedione	25	-		TWA (8 h)	

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
123-54-6	pentane-2,4-dione			
Worker DNEL, long-term		inhalation	systemic	84 mg/m ³
Worker DNEL, long-term		dermal	systemic	12 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	7 mg/kg bw/day

PNEC values

CAS No	Substance	Value
123-54-6	pentane-2,4-dione	
Freshwater		0,2 mg/l
Freshwater (intermittent releases)		0,26 mg/l
Marine water		0,02 mg/l
Freshwater sediment		1,909 mg/kg
Marine sediment		0,191 mg/kg
Micro-organisms in sewage treatment plants (STP)		1,32 mg/l
Soil		0,193 mg/kg

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection

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equipment. Provide adequate ventilation as well as local exhaust at critical locations.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles
Face protection umbrella

Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact: No data available

By short-term hand contact

Trade name/designation KCL 898 Butoject®
Suitable material: Butyl caoutchouc (butyl rubber) 0,7 mm
Wearing time with occasional contact (splashes): >240 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet (>, <) supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin protection

Take off immediately all contaminated clothing and wash it before reuse.
Wear fire resistant or flame retardant clothing.
Wash hands and face before breaks and after work and take a shower if necessary.
Draw up and observe skin protection programme.

Respiratory protection

Filtering device with filter or ventilator filtering device of type: A
Wear breathing apparatus if exposed to vapours/dusts/aerosols.

Environmental exposure controls

Do not allow to enter into surface water or drains.
Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.
Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	colourless
Odour:	rancid

Changes in the physical state

Melting point/freezing point:	-23 °C
Boiling point or initial boiling point and boiling range:	139 °C °C
Sublimation point:	No data available
Softening point:	No data available
Pour point:	No data available
:	No data available
Flash point:	34 °C °C

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Flammability

Solid/liquid: not applicable
Gas: not applicable

Explosive properties

Vapours are heavier than air, spread along floors and form explosive mixtures with air.

Lower explosion limits: 1,7
Upper explosion limits: 11,4
Auto-ignition temperature: 340 °C °C

Self-ignition temperature

Solid: not applicable
Gas: not applicable

Decomposition temperature: not determined

pH-Value: 6,0

Viscosity / dynamic: No data available

Viscosity / kinematic: No data available

Flow time: No data available

Water solubility: 200 g/L
(at 20 °C)

Solubility in other solvents

not determined

Partition coefficient n-octanol/water: not determined

Vapour pressure: 9 hPa hPa
(at 20 °C)

Vapour pressure: not determined

Density: 0,97 g/cm³

Bulk density: No data available

Relative vapour density: not determined

9.2. Other information

Information with regard to physical hazard classes

Oxidizing properties
Not oxidising.

Other safety characteristics

Solvent separation test: No data available

Solvent content: 100

Solid content: not determined

Evaporation rate: not determined

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Flammable.
Vapours may form explosive mixtures with air.

10.2. Chemical stability

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The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Acid
Oxidising agent
Hydrogen fluoride
Amines
Amines
Isocyanate

10.4. Conditions to avoid

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Vapours can form explosive mixtures with air.

10.5. Incompatible materials

No data available

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

Toxic in contact with skin.
Toxic if inhaled.
Harmful if swallowed.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
123-54-6	pentane-2,4-dione				
	oral	LD50 760 mg/kg	Rat	Drug and Chemical Toxicology, 9, 133-146	other: as stated in report
	dermal	LD50 790 mg/kg	Rabbit	Drug and Chemical Toxicology, 9, 133-146	other: as reported in test report
	inhalation (4 h) vapour	LC50 1224 mg/l	Rat	Study report (1984)	OECD Guideline 403
	inhalation dust/mist	ATE 0,5 mg/l			

Irritation and corrosivity

Based on available data, the classification criteria are not met.

Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

STOT-single exposure

Based on available data, the classification criteria are not met.

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STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

Further information

No data available

SECTION 12: Ecological information

12.1. Toxicity

The product is not: Ecotoxic.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
123-54-6	pentane-2,4-dione					
	Acute fish toxicity	LC50 104 mg/l	96 h	Pimephales promelas	Center of Lake Superior Environmental St	OECD Guideline 203
	Acute algae toxicity	ErC50 mg/l 83,22	72 h	Pseudokirchneriella subcapitata	Study report (2010)	OECD Guideline 201
	Acute crustacea toxicity	EC50 75 mg/l	48 h	Daphnia magna	Environ. Toxicol. Chem. 5, 393-398. (198	other: ASTM Standard D4229-84 of 1984
	Fish toxicity	NOEC 10 mg/l	34 d	Pimephales promelas	Study report (2012)	OECD Guideline 210
	Crustacea toxicity	NOEC 18 mg/l	21 d	Daphnia magna	Study report (2012)	OECD Guideline 211
	Acute bacteria toxicity	(EC50 mg/l) 107,6	3 h	activated sludge of a predominantly domestic sewage	Study report (2010)	OECD Guideline 209

12.2. Persistence and degradability

The product has not been tested.

12.3. Bioaccumulative potential

The product has not been tested.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
123-54-6	pentane-2,4-dione	0,68

BCF

CAS No	Chemical name	BCF	Species	Source
123-54-6	pentane-2,4-dione	3,16		Calculation (2000)

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12.4. Mobility in soil

The product has not been tested.

12.5. Results of PBT and vPvB assessment

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

The product has not been tested.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

No information available.

Further information

Discharge into the environment must be avoided.

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

Send to a physico-chemical treatment facility under observation of official regulations.

Do not empty into drains.

Contaminated packaging

This material and its container must be disposed of as hazardous waste. Handle contaminated packages in the same way as the substance itself.

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

SECTION 14: Transport information

Land transport (ADR/RID)

<u>14.1. UN number or ID number:</u>	UN 2310
<u>14.2. UN proper shipping name:</u>	PENTANE-2,4-DIONE
<u>14.3. Transport hazard class(es):</u>	3
<u>14.4. Packing group:</u>	III
Hazard label:	3+6.1
Classification code:	FT1
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	3
Hazard No:	36
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

<u>14.1. UN number or ID number:</u>	UN 2310
<u>14.2. UN proper shipping name:</u>	PENTANE-2,4-DIONE
<u>14.3. Transport hazard class(es):</u>	3
<u>14.4. Packing group:</u>	III
Hazard label:	3+6.1
Classification code:	FT1
Special Provisions:	802
Limited quantity:	5 L
Excepted quantity:	E1

Marine transport (IMDG)

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14.1. UN number or ID number:	UN 2310
14.2. UN proper shipping name:	PENTANE-2,4-DIONE
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3+6.1
Special Provisions:	-
Limited quantity:	5 L
Excepted quantity:	E1
EmS:	F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 2310
14.2. UN proper shipping name:	PENTANE-2,4-DIONE
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3+6.1
Limited quantity Passenger:	2 L
Passenger LQ:	Y343
Excepted quantity:	E1
IATA-packing instructions - Passenger:	355
IATA-max. quantity - Passenger:	60 L
IATA-packing instructions - Cargo:	366
IATA-max. quantity - Cargo:	220 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: Combustible liquid. Toxic.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40

Information according to 2012/18/EU (SEVESO III): H2 ACUTE TOXIC

Additional information: P5c

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 1 - slightly hazardous to water

Skin resorption/Sensitization: Permeates easily through outer skin and causes poisoning.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Safety Data Sheet

according to Regulation (EC) No 1907/2006

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Abbreviations and acronyms

ADR: Accord européen sur le transport des marchandises dangereuses par Route
(European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service
LC50: Lethal concentration, 50%
LD50: Lethal dose, 50%

Relevant H and EUH statements (number and full text)

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H311+H331	Toxic in contact with skin or if inhaled.
H331	Toxic if inhaled.

Further Information

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.