

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Cumene for synthesis

Revision date: 24.06.2022

Product code: 22577

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

1.1. Product identifier

Cumene for synthesis

CAS No: 98-82-8
Index No: 601-024-00-X
EC No: 202-704-5

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

Use of the substance/mixture

Laboratory chemicals

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
e-mail: info@berndkraft.de
Contact person: Abteilung Produktsicherheit
e-mail: produktsicherheit@berndkraft.de
Internet: www.berndkraft.de
Responsible Department: Abteilung Produktsicherheit
Telefax: 0203/5194-290
Telephone: 0203/5194-107/117

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

A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 3; H226
Carc. 1B; H350
STOT SE 3; H335
Asp. Tox. 1; H304
Aquatic Chronic 2; H411

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

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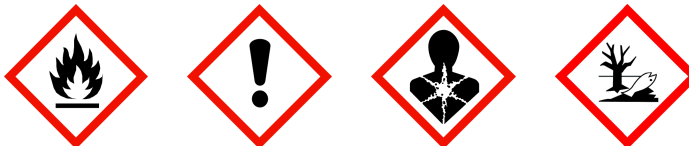
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Pictograms:



Hazard statements

H226 Flammable liquid and vapour.
 H304 May be fatal if swallowed and enters airways.
 H335 May cause respiratory irritation.
 H350 May cause cancer.
 H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

P201 Obtain special instructions before use.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/protective clothing/eye protection/face protection.
 P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
 P308+P313 IF exposed or concerned: Get medical advice/attention.
 P331 Do NOT induce vomiting.
 P391 Collect spillage.

Special labelling of certain mixtures

Restricted to professional users.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₆H₅CH(CH₃)₂
 Molecular weight: 120,19 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	Index No
	REACH No	
	Classification (Regulation (EC) No 1272/2008)	
98-82-8	isopropylbenzene	100 %
	202-704-5	601-024-00-X
	Flam. Liq. 3, Carc. 1B, STOT SE 3, Asp. Tox. 1, Aquatic Chronic 2; H226 H350 H335 H304 H411	

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		
98-82-8	202-704-5	isopropylbenzene	100 %
	dermal: LD50 = > 3160 mg/kg; oral: LD50 = 2700 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

Self-protection of the first aider

After inhalation

Provide fresh air.
If breathing is irregular or stopped, administer artificial respiration.
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 contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately. Remove contact lenses, if present and easy to do. Continue rinsing.

After ingestion

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

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

Irritant
Cough
Dyspnoea
Gastrointestinal complaints
Dizziness
Anaesthetic state
Agitation
Spasms
Headache
May cause drowsiness or dizziness.
Has degreasing effect on the skin.

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

Carbon dioxide (CO₂)
Foam
Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquids
Vapours are heavier than air, spread along floors and form explosive mixtures with air.
Beware of reignition.
Hazardous combustion products
Heating causes rise in pressure with risk of bursting.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.
In case of fire and/or explosion do not breathe fumes.
Avoid contact with skin, eyes and clothes.

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Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
Move undamaged containers from immediate hazard area if it can be done safely.
Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.
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.

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Advice on protection against fire and explosion

Take action to prevent static discharges. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.
Draw up and observe skin protection programme.
Wash hands and face before breaks and after work and take a shower if necessary.
If handled uncovered, arrangements with local exhaust ventilation have to be used.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep in a cool, well-ventilated place.
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
storage temperature < +30°C

Further information on storage conditions

Keep cool. Protect from sunlight.
Keep container dry.
Store in a place accessible by authorized persons only.

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
98-82-8	Isopropyl benzene	20	100		TWA (8 h)	
		50	250		STEL (15 min)	

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
98-82-8	isopropylbenzene			
	Worker DNEL, long-term	inhalation	systemic	100 mg/m ³
	Worker DNEL, acute	inhalation	local	250 mg/m ³
	Worker DNEL, long-term	dermal	systemic	15,4 mg/kg bw/day
	Consumer DNEL, long-term	inhalation	systemic	16,6 mg/m ³
	Consumer DNEL, long-term	dermal	systemic	1,2 mg/kg bw/day
	Consumer DNEL, long-term	oral	systemic	5 mg/kg bw/day

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PNEC values

CAS No	Substance	Value
Environmental compartment		
98-82-8	isopropylbenzene	
Freshwater		0,035 mg/l
Freshwater (intermittent releases)		0,012 mg/l
Marine water		0,004 mg/l
Freshwater sediment		3,22 mg/kg
Marine sediment		0,322 mg/kg
Micro-organisms in sewage treatment plants (STP)		200 mg/l
Soil		0,624 mg/kg

8.2. Exposure controls

Appropriate engineering controls

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

If handled uncovered, arrangements with local exhaust ventilation have to be used.

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
Trade name/designation KCL 890 Vitoject®
Suitable material: FKM (fluoro rubber) 0,7 mm
Wearing time with permanent contact: > 480 min

By short-term hand contact
Trade name/designation KCL 730 Camatril® Velours
Suitable material: NBR (Nitrile rubber) 0,4 mm
Wearing time with occasional contact (splashes): > 30 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

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

Thermal hazards

No data available

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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:	like: Hydrocarbons, aromatic
Odour threshold:	No data available

Changes in the physical state

Melting point/freezing point:	-96 °C
Boiling point or initial boiling point and boiling range:	152,39 °C
Sublimation point:	No data available
Softening point:	No data available
Pour point:	No data available
:	No data available
Flash point:	ca. 31 °C

Flammability

Solid/liquid:	No data available
Gas:	No data available

Explosive properties

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

Lower explosion limits:	0,9 vol. %
Upper explosion limits:	6,5 vol. %
Auto-ignition temperature:	424 °C

Self-ignition temperature

Solid:	No data available
Gas:	No data available

Decomposition temperature:	No data available
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pH-Value:	No data available
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Viscosity / dynamic: (at 20 °C)	0,79 mPa·s
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Viscosity / kinematic:	No data available
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Flow time:	No data available
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Water solubility: (at 20 °C)	0,05 g/L
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Solubility in other solvents

No data available

Dissolution rate:	No data available
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Partition coefficient n-octanol/water:	No data available
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Dispersion stability:	No data available
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Vapour pressure: (at 20 °C)	4,96 hPa
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Vapour pressure:	No data available
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Density (at 20 °C):	0,86 g/cm ³
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information

Information with regard to physical hazard classes

Sustaining combustion:	No data available
Oxidizing properties	
No data available	

Other safety characteristics

Solvent separation test:	No data available
Solvent content:	100%
Solid content:	No data available
Evaporation rate:	No data available

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

In case of warming: Vapours may form explosive mixtures with air.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Oxidising agent
Nitric acid

10.4. Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

10.5. Incompatible materials

Rubber articles

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

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

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CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
98-82-8	isopropylbenzene				
	oral	LD50 mg/kg 2700	Rat	Other company data (1978)	OECD Guideline 401
	dermal	LD50 mg/kg > 3160	Rabbit	Other company data (1978)	1 New Zealand albino rabbit

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

May cause cancer. (isopropylbenzene)

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

STOT-single exposure

May cause respiratory irritation. (isopropylbenzene)

STOT-repeated exposure

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

Aspiration hazard

May be fatal if swallowed and enters airways.

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

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

No data available

Further information

- Irritant
- Cough
- Dyspnoea
- Gastrointestinal complaints
- Dizziness
- Anaesthetic state
- Agitation
- Spasms
- Headache
- May cause drowsiness or dizziness.
- Has degreasing effect on the skin.

SECTION 12: Ecological information

12.1. Toxicity

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CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
98-82-8	isopropylbenzene					
	Acute fish toxicity	LC50 4,7 mg/l	96 h	Cyprinodon variegatus	Ecotoxicol. Environ. Saf. 31, 287-289 (1)	EPA OTS 797.1400
	Acute algae toxicity	ErC50 mg/l 2,01	72 h	Desmodesmus subspicatus	Study report (2010)	EU Method C.3
	Acute crustacea toxicity	EC50 mg/l 2,14	48 h	Daphnia magna	Study report (2010)	OECD Guideline 202
	Fish toxicity	NOEC mg/l 0,38	28 d	D. rerio and P. promelas	European Chemicals Bureau (2001)	Chronic NOEC was calculated by the rappo
	Crustacea toxicity	NOEC mg/l 0,35	21 d	Daphnia magna	Draft study report (incomplete) (1998)	OECD Guideline 211
	Acute bacteria toxicity	(EC50 mg/l) > 2000	3 h	activated sludge of a predominantly domestic sewage	Study report (2010)	EU Method C.11

12.2. Persistence and degradability

86 %; 28 d
ISO 10708
(IUCLID)

12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
98-82-8	isopropylbenzene	3,55

BCF

CAS No	Chemical name	BCF	Species	Source
98-82-8	isopropylbenzene	94,69		Unpublished calculat

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

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

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.
No data available

12.7. Other adverse effects

Do not allow to enter into surface water or drains.

Further information

Avoid release to the environment.

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.

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Do not empty into drains.

Contaminated packaging

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)

14.1. UN number or ID number:	UN 1918
14.2. UN proper shipping name:	ISOPROPYLBENZENE
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Classification code:	F1
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	3
Hazard No:	30
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 1918
14.2. UN proper shipping name:	ISOPROPYLBENZENE
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Classification code:	F1
Limited quantity:	5 L
Excepted quantity:	E1

Marine transport (IMDG)

14.1. UN number or ID number:	UN 1918
14.2. UN proper shipping name:	ISOPROPYLBENZENE
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Special Provisions:	-
Limited quantity:	5 L
Excepted quantity:	E1
EmS:	F-E, S-E

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 1918
14.2. UN proper shipping name:	ISOPROPYLBENZENE
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Limited quantity Passenger:	10 L
Passenger LQ:	Y344
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

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ENVIRONMENTALLY HAZARDOUS: Yes
Danger releasing substance: isopropylbenzene

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): E2 Hazardous to the Aquatic Environment

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

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 2,4,7,8,11,12,15.

Relevant H and EUH statements (number and full text)

H226 Flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.
H335 May cause respiratory irritation.
H350 May cause cancer.
H411 Toxic to aquatic life with long lasting effects.

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. The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.