

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 25.02.2013

Version 8.8

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

1.1 Product identifier

Catalogue No.	820560
Product name	Isopropyl acetate for synthesis
REACH Registration Number	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.

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0
Responsible Department	EQ-RS * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number

Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225

Eye irritation, Category 2, H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

F	Highly flammable	R11
Xi	Irritant	R36

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

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Hazard statements

H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H336 May cause drowsiness or dizziness.
EUH066 Repeated exposure may cause skin dryness or cracking.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233 Keep container tightly closed.

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Reduced labelling (≤125 ml)



Hazard pictograms



Signal word
Danger



Index-No. 607-024-00-6

Labelling (67/548/EEC or 1999/45/EC)

<i>Symbol(s)</i>	 F  Xi	Highly flammable Irritant
<i>R-phrases(s)</i>	11-36-66-67	Highly flammable. Irritating to eyes. Repeated exposure may cause skin dryness or cracking. Vapours may cause drowsiness and dizziness.
<i>S-phrases(s)</i>	16-26-29-33	Keep away from sources of ignition - No smoking. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Do not empty into drains. Take precautionary measures against static discharges.

EC-No. 203-561-1 EC Label

Reduced labelling (≤125 ml)

<i>Symbol(s)</i>	 F  Xi	Highly flammable Irritant
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2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ COOCH(CH ₃) ₂	C ₅ H ₁₀ O ₂ (Hill)
CAS-No.	108-21-4	
Index-No.	607-024-00-6	
EC-No.	203-561-1	
Molar mass	102,13 g/mol	

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Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
isopropyl acetate (<= 100 %)		
108-21-4	*)	Flammable liquid, Category 2, H225 Eye irritation, Category 2, H319 Specific target organ toxicity - single exposure, Category 3, H336

*) 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.

For the full text of the H-Statements mentioned in this Section, see Section 16.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
isopropyl acetate (<= 100 %)	
108-21-4	F, Highly flammable; R11 Xi, Irritant; R36 R66 R67

For the full text of the R-phrases mentioned in this Section, see Section 16.

3.2 Mixture

not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Consult doctor if feeling unwell.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of aspiration). Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, respiratory paralysis, Drowsiness, Dizziness, narcosis, Headache, drowsiness

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

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Forms explosive mixtures with air at ambient temperatures.
Pay attention to flashback.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Cool closed containers exposed to fire with water spray. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Work under hood. Do not inhale substance/mixture.

Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place.

Store at +15°C to +25°C.

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7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

splash contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 60 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (splash contact). 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).

Other protective equipment

protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: filter ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not empty into drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

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Form	liquid
Colour	colourless
Odour	stinging
Odour Threshold	No information available.
pH	No information available.
Melting point	-73 °C
Boiling point/boiling range	88 - 90 °C at 1.013 hPa
Flash point	4 °C Method: DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,8 %(V)
Upper explosion limit	8 %(V)
Vapour pressure	61 hPa at 20 °C
Relative vapour density	3,52
Relative density	0,87 g/cm ³ at 20 °C
Water solubility	31 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 1,02 (HSDB)
	Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0,525 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

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Ignition temperature	460 °C Method: DIN 51794
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SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, alkalines, Bases

10.4 Conditions to avoid

Warming.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.5 Incompatible materials

various plastics

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 rat: 6.750 mg/kg (RTECS)

absorption

Symptoms: Risk of aspiration upon vomiting., Pulmonary failure possible after aspiration of vomit.

Acute inhalation toxicity

LC50 rat: 50,6 mg/l; 8 h (IUCLID)

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 rabbit: > 20.000 mg/kg (IUCLID)

Skin irritation

rabbit

Result: slight irritation

(IUCLID)

Repeated exposure may cause skin dryness or cracking.

Eye irritation

rabbit

Result: Eye irritation

(IUCLID)

Causes serious eye irritation.

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Sensitisation

Sensitisation test: guinea pig
Result: negative
(IUCLID)

Germ cell mutagenicity

Genotoxicity in vitro

Ames test
Result: negative
(IUCLID)

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

After absorption of large quantities:

Systemic effects:

lack of appetite, Headache, drowsiness, Drowsiness, Dizziness, narcosis

Possible damages:

respiratory paralysis

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 *Leuciscus idus* (Golden orfe): 265 mg/l; 48 h (Lit.)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia magna* (Water flea): 4.150 mg/l; 24 h (IUCLID)

Toxicity to algae

IC5 *Scenedesmus quadricauda* (Green algae): 165 mg/l; 8 d (IUCLID)

Toxicity to bacteria

EC5 *Pseudomonas putida*: 190 mg/l; 16 h (IUCLID)

12.2 Persistence and degradability

Ratio BOD/ThBOD

BOD5 61 %

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,02

(HSDB)

Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

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12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 1220
14.2 Proper shipping name	ISOPROPYL ACETATE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1220
14.2 Proper shipping name	ISOPROPYL ACETATE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 1220
14.2 Proper shipping name	ISOPROPYL ACETATE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

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EU regulations

Major Accident Hazard	96/82/EC
Legislation	Highly flammable 7b Quantity 1: 5.000 t Quantity 2: 50.000 t

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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National legislation

Storage class	3
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15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.

Full text of R-phrases referred to under sections 2 and 3

R11	Highly flammable.
R36	Irritating to eyes.
R66	Repeated exposure may cause skin dryness or cracking.
R67	Vapours may cause drowsiness and dizziness.

Training advice

Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.