

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 29.01.2014

Version 11.1

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

1.1 Product identifier

Catalogue No.	803649
Product name	N,N'-Diisopropylcarbodiimide 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.
CAS-No.	693-13-0

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	LS-QHC * 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 3, H226
Acute toxicity, Category 2, Inhalation, H330
Serious eye damage, Category 1, H318
Respiratory sensitisation, Category 1, H334
Skin sensitisation, Category 1, H317

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

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

	Flammable	R10
T+	Very toxic	R26
Xi	Irritant	R41
	Sensitising	R42/43

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

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

H330 Fatal if inhaled.

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat.

P280 Wear protective gloves.

P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

H330 Fatal if inhaled.

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statements

P280 Wear protective gloves.

P280 Wear eye protection.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

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2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$(\text{CH}_3)_2\text{CHN}=\text{C}=\text{NCH}(\text{CH}_3)_2$	$\text{C}_7\text{H}_{14}\text{N}_2$ (Hill)
EC-No.	211-743-7	
Molar mass	126,2 g/mol	

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

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
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N,N'-diisopropylcarbodiimide ($\leq 100\%$)

693-13-0	*)	
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Flammable liquid, Category 3, H226
Acute toxicity, Category 2, H330
Serious eye damage, Category 1, H318
Respiratory sensitisation, Category 1, H334
Skin sensitisation, Category 1, H317

*) 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
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N,N'-diisopropylcarbodiimide ($\leq 100\%$)

693-13-0	R10 T+, Very toxic; T+; R26 Xi, Irritant; Xi; R41 R42/43
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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

General advice

First aider needs to protect himself.

After inhalation: fresh air. If breathing stops: immediately apply artificial respiration, if necessary oxygen. Immediately call in physician.

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

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

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After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Allergic reactions, Nausea, Vomiting, Headache
Risk of serious damage to eyes.

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

Water, 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.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

Hydrogen cyanide (hydrocyanic acid), nitrogen oxides

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. Suppress (knock down) gases/vapours/mists with a water spray jet. 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. Keep away from heat and sources of ignition. Ensure adequate ventilation. 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 carefully 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.

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SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols. Keep workplace dry. Do not allow product to come into contact with water.

Observe label precautions.

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.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

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

Tightly fitting safety goggles

Hand protection

splash contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 10 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).

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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

Flame retardant antistatic protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Empfohlener Filtertyp: Respirator.

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

Form	liquid
Colour	colourless to light yellow
Odour	unpleasant
Odour Threshold	No information available.
pH	No information available.
Melting point	No information available.
Boiling point/boiling range	145 - 148 °C at 1.013 hPa
Flash point	33 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.

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Relative density	0,81 g/cm ³ at 20 °C
Water solubility	at 20 °C (decomposition)
Partition coefficient: n-octanol/water	No information available.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

10.2 Chemical stability

sensitive to moisture

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents, acids

can decompose violently in contact with:

Water

10.4 Conditions to avoid

Heating.

Exposure to moisture.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

Symptoms: Nausea, Vomiting, Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity

LC50 rat: 0,1 mg/l; 4 h (External MSDS)

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Rapid absorption.
Symptoms: Possible damages: mucosal irritations

Acute dermal toxicity
This information is not available.

Skin irritation
Possible damages: slight irritation

Eye irritation
Causes serious eye damage.

Sensitisation
May cause an allergic skin reaction.
May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Germ cell mutagenicity
Genotoxicity in vitro
Mutagenicity (mammal cell test):
Result: positive
(Lit.)

Ames test
Result: negative
(Lit.)

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
This information is not available.

Specific target organ toxicity - repeated exposure
This information is not available.

Aspiration hazard
This information is not available.

11.2 Further information

After absorption:
Headache
Other dangerous properties can not be excluded.
This substance should be handled with particular care.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

No information available.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

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

12.6 Other adverse effects

Additional ecological information

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 2929
14.2 Proper shipping name	TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (N,N'-DIISOPROPYLCARBODIIMIDE)
14.3 Class	6.1 (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 2929
14.2 Proper shipping name	TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (N,N'-DIISOPROPYLCARBODIIMIDE)
14.3 Class	6.1 (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 2929
14.2 Proper shipping name	TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (N,N'-DIISOPROPYLCARBODIIMIDE)
14.3 Class	6.1 (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

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SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard	96/82/EC
Legislation	Very toxic
	1
	Quantity 1: 5 t
	Quantity 2: 20 t

	96/82/EC
	Flammable.
	6
	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. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals	not regulated
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Substances of very high concern (SVHC)	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).
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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.

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SECTION 16. Other information

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

H226	Flammable liquid and vapour.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.


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

R10	Flammable.
R26	Very toxic by inhalation.
R41	Risk of serious damage to eyes.
R42/43	May cause sensitisation by inhalation and skin contact.

Training advice

Provide adequate information, instruction and training for operators.

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

Symbol(s)	 T+	Very toxic
R-phrases(s)	10-26-41-42/43	Flammable. Very toxic by inhalation. Risk of serious damage to eyes. May cause sensitisation by inhalation and skin contact.
S-phrases(s)	23-26-28-36/37/39-45	Do not breathe vapour. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. After contact with skin, wash immediately with plenty of water. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).
EC-No.	211-743-7	

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.