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

Anisole ≥99 %, for synthesis

article number: **4417**Version: **6.0 en**date of compilation: 2016-03-10
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Version: (5)



1.1 Product identifier

Identification of the substance Anisole ≥99 %, for synthesis

Article number 4417

EC number 202-876-1 CAS number 100-66-3

Alternative name(s) Methoxybenzene

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

Relevant identified uses: Laboratory chemical

Laboratory and analytical use

Uses advised against: Do not use for private purposes (household).

Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 **e-mail:** sicherheit@carlroth.de **Website:** www.carlroth.de

Competent person responsible for the safety data Department Health, Safety and Environment

sheet:

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	3	Flam. Liq. 3	H226
3.8D	Specific target organ toxicity - single exposure (narcotic effects, drowsiness)	3	STOT SE 3	H336

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Supplemental hazard information

Code	Supplemental hazard information
EUH066	repeated exposure may cause skin dryness or cracking

For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

Signal word Warning

Pictograms

GHS02, GHS07



Hazard statements

H226 Flammable liquid and vapour H336 May cause drowsiness or dizziness

Precautionary statements

Precautionary statements - prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition

sources. No smoking

Precautionary statements - storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed

Supplemental hazard information

EUH066 Repeated exposure may cause skin dryness or cracking.

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Anisole

Molecular formula C_7H_8O Molar mass $108,1~^g/_{mol}$ CAS No 100-66-3EC No 202-876-1

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritant effects, Headache, Drowsiness, Cough, Dyspnoea, Agitation, Nausea, Vomiting, Spasms, Dizziness, Drowsiness, Narcosis

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings! water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO_2)

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Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

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

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Avoid exposure.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Store in a well-ventilated place. Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ground/bond container and receiving equipment.

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

Human health values

Relevant DNELs and other threshold levels Endpoint Threshold level Protection goal, route of exposure Used in Exposure time DNEL 20 mg/m³ human, inhalatory worker (industry) chronic - systemic effects

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Environmental values

Relevant PNECs and other threshold levels

End- point			Environmental com- partment	Exposure time
PNEC	27 ^{µg} / _l	aquatic organisms	freshwater	short-term (single instance)
PNEC	2,7 ^{µg} / _l	aquatic organisms	marine water	short-term (single instance)
PNEC	30 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,745 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,074 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,133 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection.

Skin protection





hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

type of material

FKM (fluoro rubber)

material thickness

0,4 mm

breakthrough times of the glove material

>480 minutes (permeation: level 6)

Splash protection - Protective gloves

• type of material: NBR (Nitrile rubber)

• material thickness: 0,4 mm

• breakthrough times of the glove material: >30 minutes (permeation: level 2)

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other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection





Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state liquid

Colour colourless - light yellow

Odour mild sweet

Melting point/freezing point -37 °C

Boiling point or initial boiling point and boiling

range

Flammability flammable liquid in accordance with GHS criteria

153 - 156 °C

Lower and upper explosion limit 1,2 vol% (LEL) - 6,3 vol% (UEL)

Flash point 45,5 °C at 744,9 mmHg (ECHA)

Auto-ignition temperature 475 °C at 745 mmHg (ECHA)

Decomposition temperature >490 °C

pH (value) not determined Kinematic viscosity $1 \, {\rm mm^2/_s}$ at 25 °C

Dynamic viscosity 0,99 mPa s at 25 °C

Solubility(ies)

Water solubility 1,71 9 / $_{1}$ at 20 $^{\circ}$ C (ECHA)

Partition coefficient

Partition coefficient n-octanol/water (log value): 2,62 (30 °C) (ECHA)

Vapour pressure 4,7 hPa at 25 °C

Density and/or relative density

Density $0.99 \, ^{9}/_{cm^3}$ Relative vapour density $3.7 \, (air = 1)$

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not relevant (liquid)

Other safety parameters

Particle characteristics

Oxidising properties none

9.2 Other information

Information with regard to physical hazard

classes:

There is no additional information.

Other safety characteristics:

Gas group (explosion group)

Maximum Experimental Safe Gap value; 0,5 mm ≤ $MESG \leq 0.9 \text{ mm}$

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition. May form explosive peroxides.

Risk of ignition. Vapours may form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser, Strong alkali, Strong acid

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Keep away from heat. Decompostion takes place from temperatures above: >490 °C.

10.5 Incompatible materials

Rubber articles, different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5. Peroxides.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful if swallowed.

Acute toxicity

Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	3.700 ^{mg} / _{kg}	rat		TOXNET

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Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

vomiting, nausea

• If in eyes

slightly irritant but not relevant for classification

• If inhaled

headache, drowsiness, cough, Dyspnoea, fatigue, narcosis

• If on skin

has degreasing effect on the skin, Frequently or prolonged contact with skin may cause dermal irritation

Other information

Other adverse effects: Liver and kidney damage

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

11.3 Information on other hazards

There is no additional information.



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SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
EC50	27 ^{mg} / _l	aquatic invertebrates	ECHA	48 h
ErC50	47 ^{mg} / _l	algae	ECHA	72 h

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2,515 ^{mg}/_{mg} Theoretical Carbon Dioxide: 2,849 ^{mg}/_{mg}

Biodegradation

The substance is readily biodegradable.

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	2,62 (30 °C) (ECHA)
, ,	

12.4 Mobility in soil

Henry's law constant	27,77 ^{Pa m³} / _{mol} at 25 °C (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

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13.2 Relevant provisions relating to waste

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

Properties of waste which render it hazardous

HP 3 flammable

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

14.1 UN number or ID number

ADRRID	UN 2222
IMDG-Code	UN 2222
ICAO-TI	UN 2222

14.2 UN proper shipping name

ADRRID	ANISOLE
IMDG-Code	ANISOLE
ICAO-TI	Anisole

14.3 Transport hazard class(es)

ADRRID	3
IMDG-Code	3
ICAO-TI	3

14.4 Packing group

ADRRID	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

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Agreement concerning the International Carriage of Dangerous Goods by Road (ADR)Additional information

Proper shipping name ANISOLE

Particulars in the transport document UN2222, ANISOLE, 3, III, (D/E)

Classification code F1
Danger label(s) 3



Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information

Classification code F1

Danger label(s) 3



Excepted quantities (EQ) E1
Limited quantities (LQ) 5 L
Transport category (TC) 3
Hazard identification No 30

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name ANISOLE

Particulars in the shipper's declaration UN2222, ANISOLE, 3, III, 45,5°C c.c.

Marine pollutant Danger label(s) 3



Special provisions (SP)
Excepted quantities (EQ) E1

Limited quantities (LQ) 5 L

EmS F-E, S-D

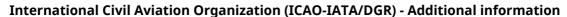
Stowage category A

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Proper shipping name Anisole

Particulars in the shipper's declaration UN2222, Anisole, 3, III

Danger label(s) 3



Excepted quantities (EQ) E1

Limited quantities (LQ) 10 L

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture Relevant provisions of the European Union (EU)

Seveso Directive

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories		(tonnes) for the ap- and upper-tier re- ments	Notes
P5c	flammable liquids (cat. 2, 3)	5.000	50.000	51)

Notation

51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b

Deco-Paint Directive

VOC content	100 %
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Industrial Emissions Directive (IED)

VOC content	100 %
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Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

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Regulation concerning the export and import of hazardous chemicals (PIC)

Regulation on persistent organic pollutants (POP)

not listed

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
Anisole	this product meets the criteria for classi- fication in accordance with Regulation No 1272/2008/EC		3
Anisole	flammable / pyrophoric		40

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC CSCL-ENCS DSL ECSI

Australian Inventory of Industrial Chemicals
List of Existing and New Chemical Substances (CSCL-ENCS)
Domestic Substances List (DSL)
EC Substance Inventory (EINECS, ELINCS, NLP)
Inventory of Existing Chemical Substances Produced or Imported in China

National Inventory of Chemical Substances Korea Existing Chemicals Inventory

NCI National Chemical Inventory
NZIOC New Zealand Inventory of Chemicals
PICCS Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg. REACH registered substances

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Legend

Taiwan Chemical Substance Inventory Toxic Substance Control Act TCSI TSCA

15.2 Chemical safety assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3	Endocrine disrupting properties: Does not contain an endocrine disruptor (EDC) in a concentration of ≥ 0,1%.	Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code

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Abbr.	Descriptions of used abbreviations
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula- tions concerning the International carriage of Dangerous goods by Rail)
UEL	Upper explosion limit (UEL)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H226	Flammable liquid and vapour.
H336	May cause drowsiness or dizziness.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.

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