according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



date of compilation: 2016-03-10

Anisole ≥99 %, for synthesis

article number: **4417** Version: **1.0 en**

SECTION 1: Identification of the substance/mixture and of the company/undertaking				
1.1	Product identifier			
	Identification of the substance	Anisole		
	Article number	4417		
	Registration number (REACH)	This information is not available.		
	EC number	202-876-1		
	CAS number	100-66-3		
1.2	2 Relevant identified uses of the substance or mixture and uses advised against			
	Identified uses:	laboratory chemical		
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 sheet	: Department Health, Safety and Environment		
	e-mail (competent person)	: sicherheit@carlroth.de		
1.4	Emergency telephone number			
	Emergency information service	Poison Centre Munich: +49/(0)89 19240		

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Classification acc. to GHS			
Section	Hazard class	Hazard class and cat- egory	Hazard state- ment
2.6	flammable liquid	(Flam. Liq. 3)	H226

Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

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2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word Warning

Pictograms



Hazard statements

H226 Flammable liquid and vapour.

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.

Labelling of packages where the contents do not exceed 125 ml Signal word: Warning Symbol(s)



2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Methoxybenzene
EC number	202-876-1
CAS number	100-66-3
Molecular formula	C ₇ H ₈ O
Molar mass	108,1 ^g / _{mol}

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

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. Do not induce vomiting. Aspiration hazard. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed Irritant effects, Headache, Cough, Dyspnoea, Agitation, Nausea, Vomiting, Spasms

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 fire-fighting measures to the fire surroundings water spray, foam, dry extinguishing powder, carbon dioxide (CO2)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours can 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

Vapours are heavier than air. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

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

6.2 Environmental precautions

Keep away from drains, surface and ground water. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

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

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provide adequate ventilation. When not in use, keep containers tightly closed.

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.

7.2 Conditions for safe storage, including any incompatibilities

Store in a well-ventilated place. Keep container tightly closed. Keep away from sources of heat (e.g. hot surfaces), sparks and open flames.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

• Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C.

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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) No data available.

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

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

• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	27 μg/l	freshwater	short-term (single instance)
PNEC	2,7 µg/l	marine water	short-term (single instance)
PNEC	30 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,745 mg/kg	freshwater sediment	short-term (single instance)
PNEC	0,074 mg/kg	marine sediment	short-term (single instance)
PNEC	0,133 mg/kg	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.

type of material

FKM (fluoro rubber)

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



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material thickness

- 0,7mm.
- breakthrough times of the glove material
- >480 minutes (permeation: level 6)

Splash protection - Protective gloves

- Type of material
- NBR (Nitrile rubber).
- Material thickness
- 0,4mm.

Breakthrough times of the glove material

>30 minutes (permeation: level 2).

• 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). Observe the wear time limits according GefStoffV in combination with the rules for using respiratory

protection apparatus (BGR 190).

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

Appearance	
Physical state	liquid (fluid)
Colour	colourless - light yellow
Odour	mild sweet
Odour threshold	No data available
Other physical and chemical parameters	
pH (value)	This information is not available.
Melting point/freezing point	-37 °C
Initial boiling point and boiling range	153 - 156 °C
Flash point	44 °C
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
Explosive limits	
 lower explosion limit (LEL) 	0,34 vol%
 upper explosion limit (UEL) 	6,3 vol%
Explosion limits of dust clouds	not relevant
Vapour pressure	3,2 hPa at 20 °C
Density	0,99 ^g / _{cm³}

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Vapour density	3,7 air = 1
Bulk density	Not applicable
Relative density	Information on this property is not available.
Solubility(ies)	
Water solubility	1,7 ^g / _l at 20 °C
Partition coefficient	
n-octanol/water (log KOW)	2,11 (Lit.) (exp.)
Auto-ignition temperature	475 °C
Decomposition temperature	>490 °C
Viscosity	
• dynamic viscosity	1,42 mPa s at 15 °C
Explosive properties	none
Oxidising properties	none

9.2 Other information

There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

In case of warming: Vapours can form explosive mixtures with air. risk of ignition. May form explosive peroxides.

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.
- **10.5 Incompatible materials** There is no additional information.
- **10.6 Hazardous decomposition products** Peroxides.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
inhalation: vapour	LC50	>6,51 ^{mg} /լ/4h	rat	ECHA
oral	LD50	3.700 ^{mg} / _{kg}	rat	TOXNET

Skin corrosion/irritation

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.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

• Specific target organ toxicity - single exposure

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

• 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

gastrointestinal complaints, nausea, vomiting, presenting an aspiration hazard, Liver and kidney damage

• If in eyes

Gases/vapours, irritant

If inhaled

Inhalation of vapours or spray/mists, Irritating to respiratory system, cough, Dyspnoea

• If on skin

causes slight to moderate irritation

Other information

None

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



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SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
EC50	27 ^{mg} /լ	daphnia magna	ECHA	48 hours
LC50	>1 ^{mg} / _l	zebra fish (Danio rerio)	ECOTOX Database	96 hours
ErC50	47 ^{mg} /l	algae	ECHA	72 hours

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
NOEC	300 ^{mg} /l	microorganisms	ECHA	3 h

12.2 Process of degradability

The substance is readily biodegradable. Theoretical Oxygen Demand: 2,52 ^g/_g Theoretical Carbon Dioxide: 2,849 ^{mg}/_{mg}

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms. n-octanol/water (log KOW)

12.4 Mobility in soil

Data are not available. Henry's law constant

12.5 Results of PBT and vPvB assessment Data are not available.

12.6 Other adverse effects

Hazardous to water.

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.

2,11

27,77 Pa m³/mol at 25 °C

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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.

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.

SEC	SECTION 14: Transport information			
14.1	UN number	2222		
14.2	UN proper shipping name	ANISOLE		
	Hazardous ingredients	Anisole		
14.3	Transport hazard class(es)			
	Class	3 (flammable liquids)		
14.4	Packing group	III (substance presenting low danger)		
14.5	Environmental hazards	NONE (non-environmentally hazardous acc. to the danger- ous goods regulations)		
14.6	Special precautions for user			
447	Provisions for dangerous goods (ADR) should be co			
14.7	Transport in bulk according to Annex II of MARI The cargo is not intended to be carried in bulk.	POL and the IBC Code		
14.8	-			
	• Transport of dangerous goods by road, rail and	d inland waterway (ADR/RID/ADN)		
	UN number	2222		
	Proper shipping name	ANISOLE		
	Particulars in the transport document	UN2222, ANISOLE, 3, III, (D/E)		
	Class	3		
	Classification code	F1		
	Packing group	III		
	Danger label(s)	3		
	3			
	Excepted quantities (EQ)	E1		
	Limited quantities (LQ)	5 L		
	Transport category (TC)	3		
	Tunnel restriction code (TRC)	D/E		
	Hazard identification No	30		
	Emergency Action Code	3Y		

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• International Maritime Dangerous Goods Code (IMDG)		
UN number	2222	
Proper shipping name	ANISOLE	
Particulars in the shipper's declaration	UN2222, ANISOLE, 3, III, 44°C c.c.	
Class	3	
Packing group	III	
Danger label(s)	3	
Special provisions (SP)	-	
Excepted quantities (EQ)	E1	
Limited quantities (LQ)	5 L	
EmS	F-E, S-D	
Stowage category	A	

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)

• **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)** Not listed.

• Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS) Not listed.

• **Regulation 850/2004/EC on persistent organic pollutants (POP)** Not listed.

• Restrictions according to REACH, Annex XVII

not listed

• List of substances subject to authorisation (REACH, Annex XIV)

not listed

Seveso Directive

2012/18/EU (Seveso III)					
Νο	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the plication of lower and upper-tier r quirements	ap- Notes e-		
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

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• Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)

VOC content

100 %

• Directive on industrial emissions (VOCs, 2010/75/EU)

VOC content

100 %

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

15.2 Chemical Safety Assessment

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

SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations			
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Wa-terways)			
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)			
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)			
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures			
CMR	Carcinogenic, Mutagenic or toxic for Reproduction			
DMEL	Derived Minimal Effect Level			
DNEL	Derived No-Effect Level			
EINECS	European Inventory of Existing Commercial Chemical Substances			
ELINCS	European List of Notified Chemical Substances			
EmS	Emergency Schedule			
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations			
IMDG	International Maritime Dangerous Goods Code			
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant)			
NLP	No-Longer Polymer			
РВТ	Persistent, Bioaccumulative and Toxic			
PNEC	Predicted No-Effect Concentration			

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Abbr.	Descriptions of used abbreviations	
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals	
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)	
VOC	Volatile Organic Compounds	
vPvB	very Persistent and very Bioaccumulative	

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EÚ GHS)

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

Code	Text
H226	flammable liquid and vapour

Disclaimer

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.