SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Revision Date 27.04.2011 Version 7.0

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

1.1 Product identifier

Catalogue No.	802400
Product name	3-Bromotoluene 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).

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 2, H225
Acute toxicity, Category 3, Inhalation, H331
Chronic aquatic toxicity, Category 2, H411

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

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

Xn	Harmful	R20
N	Dangerous for the environment	R51/53

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

Hazard statements
H225 Highly flammable liquid and vapour.
H331 Toxic if inhaled.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P223 Keep away from any possible contact with water, because of violent reaction and possible flash fire.
P262 Do not get in eyes, on skin, or on clothing.
P273 Avoid release to the environment.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.
P403 + P235 Store in a well-ventilated place. Keep cool.

Reduced labelling (≤125 ml)
Hazard pictograms

Signal word
Danger

Hazard statements
H331 Toxic if inhaled.

Precautionary statements
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

CAS-No. 591-17-3

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

Symbol(s)	Xn	Harmful
	N	Dangerous for the environment
R-phrase(s)	20-51/53	Harmful by inhalation. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
S-phrase(s)	24/25-61	Avoid contact with skin and eyes. Avoid release to the environment. Refer to special instructions/ Safety data sheets.

EC-No. 209-702-3

Reduced labelling (≤125 ml)

Symbol(s)	Xn	Harmful
	N	Dangerous for the environment
R-phrase(s)	20	Harmful by inhalation.

2.3 Other hazards
None known.

SECTION 3. Composition/information on ingredients

Formula	3-(Br)$C_6H_4CH_3$	C_7H_7Br (Hill)
CAS-No.	591-17-3	

EC-No. 209-702-3
Molar mass 171,03 g/mol

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. Immediately apply artificial respiration. If necessary oxygen. Immediately call in physician.

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

After eye contact: rinse out with plenty of water.

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

Diarrhoea, Nausea, Vomiting

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO_2), 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 material, 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 bromide

5.3 Advice for firefighters

Special protective equipment for fire-fighters

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

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: Avoid substance contact. Do not breathe vapours, aerosols. 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 7.2 and 10.5).
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
Work under hood. Do not inhale substance. Avoid generation of vapours/aerosols.

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.

7.2 Conditions for safe storage, including any incompatibilities
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.

Store at +15°C to +25°C.

7.3 Specific end uses
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.

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.

Eye/face protection
Safety glasses

Hand protection

full contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 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 890 Vitoject® (full contact), KCL 730 Camatril® -Velours (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
Flame retardant antistatic protective clothing

Respiratory protection
required when vapours/aerosols are generated.
Recommended Filter type: filter ABEK
The entrepeneur 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	oily to liquid
Colour	colourless
Odour	No strong odour known.
Odour Threshold	No information available.
pH	No information available.
Melting point	-40 °C
Boiling point/boiling range	184 °C

Flash point	60 °C
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	2,04 hPa at 25 °C
Relative vapour density	No information available.
Relative density	1,405 g/cm³ at 20 °C
Water solubility	0,05 g/l
Partition coefficient: n-octanol/water	log Pow: 3,41 (experimental) A remarkable bioaccumulation potential is expected (log Po/w >3). (Lit.)
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not 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

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

10.4 Conditions to avoid

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

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products
in the event of fire: See chapter 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects
Acute oral toxicity
LD50 rat: 1.540 mg/kg (RTECS)
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity
LC50 rat: 6,8 mg/l(RTECS)
Symptoms: Irritation symptoms in the respiratory tract., Inhalation may lead to the formation of oedemas in the respiratory tract.

absorption

Genotoxicity in vitro
Ames test
Result: negative
(National Toxicology Program)

Specific target organ toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Based on available data the classification criteria are not met.

11.2 Further information
After absorption of large quantities:

Nausea, Vomiting, Diarrhoea

Damage to:

Central nervous system, Cardio-vascular system

Further data:

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
Partition coefficient: n-octanol/water
log Pow: 3,41
(experimental)
A remarkable bioaccumulation potential is expected (log Po/w >3). (Lit.)

12.4 Mobility in soil
No information available.

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

Henry constant
679,7 Pa*m³/mol
Method: (calculated)
(Lit.) Distribution preferentially in air.

Additional ecological information
We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Do not allow to run into surface waters, wastewater, or soil.

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

ADR/RID
UN 1993 FLAMMABLE LIQUID, N.O.S. (3-BROMOTOLUENE), 3, III

IATA
UN 1993 FLAMMABLE LIQUID, N.O.S. (3-BROMOTOLUENE), 3, III

IMDG
UN 1993 FLAMMABLE LIQUID, N.O.S. (3-BROMOTOLUENE), 3, III
EmS F-E S-E

The transport regulations are cited according to international regulations and in the form applicable in Germany. Possible national deviations in other countries are not considered.

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	Dangerous for the environment 9b Quantity 1: 200 t Quantity 2: 500 t
Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Take note of Dir 92/85/EEC on the safety and health at work of pregnant workers.
Storage class	3

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.
H331	Toxic if inhaled.
H411	Toxic to aquatic life with long lasting effects.

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

R20	Harmful by inhalation.
R51/53	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

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.