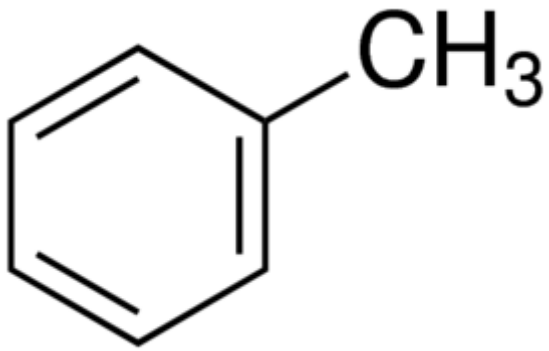
Specification Sheet

179418 Sigma-Aldrich

Toluene

ACS reagent, ≥99.5%

- **CAS Number** 108-88-3
- **Linear Formula** $C_6H_5CH_3$
- **Molecular Weight** 92.14
- **Beilstein/REAXYS Number** 635760
- **EC Number** 203-625-9
- **MDL number** MFCD00008512
- **eCl@ss** 39011102
- **PubChem Substance ID** 329751592
- **NACRES** NA.21



SKU-Pack Size	Availability	Pack Size	Price (SGD)	Quantity
179418-500ML	Estimated to ship on 07.06.2021 - FROM	500 mL	41.05	0
179418-1L	Estimated to ship on 07.06.2021 - FROM	1 L	61.49	0
179418-200L	Estimated to ship on 30.07.2021 - FROM	200 L	3,060.69	0

Properties

Related Categories	ACS Grade, ACS Grade Solvents, ACS and Reagent Grade Solvents, Amber Glass Bottles, Carbon Steel Cans with NPT Threads,
Quality Level	200
grade	**ACS reagent**
vapor density	**3.2 (vs air)**
vapor pressure	**22 mmHg (20 °C)**
	26 mmHg (25 °C)
assay	**≥99.5%**
form	**liquid**
autoignition temp.	**997 °F**
expl. lim.	**7 %**
application(s)	**microbiology: suitable**
impurities	**H_2SO_4, passes test (darkened)**
	≤0.003% *S* compounds
	≤0.030% water
evapn. residue	**≤0.0010%**
color	**APHA: ≤10**
refractive index	***n*/D 1.496 (lit.)**

bp	**110-111 °C (lit.)**
mp	**-93 °C (lit.)**
density	**0.865 g/mL at 25 °C (lit.)**
storage temp.	**room temp**
SMILES string	**Cc1ccccc1**
InChI	**1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3**
InChI key	**YXFVVABEGXRONW-UHFFFAOYSA-N**

Show Fewer Properties

Description

General description

Toluene, a flammable liquid with a pungent odor, is widely employed as organic solvent. It is widely used as a precursor for synthesizing benzene and as a solvent in the paint industry.[6] It has been reported to be a biotoxic solvent (toxic to many microorganisms at 0.1%v/v concentrations).[1] Its anaerobic biodegradation to CO_2, by the denitrifying bacterium *Thauera arornatica* has been reported.[2] It forms a syndiotactic polystyrene-toluene molecular compound. Crystal structure of this molecular compound has been investigated by X-ray diffraction studies.[3]

Application

Toluene has been employed as an solvent for the asymmetric synthesis of propargylic alcohols via addition reaction of terminal alkynes with various aldehydes in the presence of an optically active reagent, *N*-methylephedrine.[4] It may be used in the preparation of amine-capped gold nanocrystals.[5] Toluene undergoes alkylation in the presence of modified ZSM (Zeolite Socony Mobil)-5-class zeolite catalysts to form *p*-xylene with high selectivity.[8] When doped on graphene, it acts as an electron donor leading to alteration in graphene electrical properties.[7]

Packaging

1, 6×1, 2.5, 4×2.5, 4, 4×4 L in glass bottle

View returnable container options.

18, 20, 200 L in steel drum

500, 6×500 mL in glass bottle