

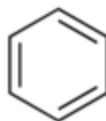
## Specification Sheet

401765 Sigma-Aldrich

## Benzene

anhydrous, 99.8%

- CAS Number [71-43-2](#)
- Empirical Formula (Hill Notation)  $C_6H_6$
- Molecular Weight 78.11
- Beilstein/REAXYS Number 969212
- EC Number [200-753-7](#)
- MDL number [MFCD00003009](#)
- PubChem Substance ID [57649920](#)
- NACRES NA.21



SKU-Pack Size	Availability	Pack Size	Price (SGD)	Quantity
401765-100ML	Available to ship on 14.04.2021 - FROM	100 mL		<input type="text" value="0"/>
401765-250ML	Available to ship on 14.04.2021 - FROM	250 mL		<input type="text" value="0"/>
401765-1L	Available to ship on 14.04.2021 - FROM	1 L		<input type="text" value="0"/>
401765-2L	Estimated to ship on 05.05.2021 - FROM	2 L		<input type="text" value="0"/>

## Properties

Related Categories	<a href="#">Anhydrous, Anhydrous Solvents, Benzene and Benzene Solutions, Returnable Containers, Solvent by Type,</a>
Quality Level	<a href="#">200</a>
grade	<b>anhydrous</b>



vapor density	2.77 (vs air)
vapor pressure	166 mmHg ( 37.7 °C)
	74.6 mmHg ( 20 °C)
assay	99.8%
form	liquid
autoignition temp.	1043 °F
expl. lim.	8 %
application(s)	toxicology assay: suitable
impurities	<0.001% water
	<0.005% water (100 mL pkg)
evapn. residue	<0.0005%
refractive index	<i>n</i> <sub>20/D</sub> 1.501 (lit.)
bp	80 °C (lit.)
mp	5.5 °C (lit.)
density	0.874 g/mL at 25 °C (lit.)
storage temp.	room temp
SMILES string	<chem>c1ccccc1</chem>
InChI	1S/C6H6/c1-2-4-6-5-3-1/h1-6H
InChI key	UHOVQNZJYSORNB-UHFFFAOYSA-N



[Show Fewer Properties](#)

## Description

### *General description*

Benzene is a six membered aromatic compound. The capability of superhalogen induced ionization of benzene molecules has been reported based on *ab initio* calculations.<sup>[2]</sup> Benzene, a commonly used industrial solvent is also an air pollutant and a potent carcinogen.<sup>[1]</sup>

### *Application*

Benzene may be used in the following processes:

- Formation of phenyl acetate by aerobic oxidation using Pd catalyst and acetic acid as solvent.<sup>[5]</sup>
- Formation of phenol by hydroxylation in the presence of mesoporous carbon nitride supported on vanadium catalyst.<sup>[3]</sup>
- As a solvent to prepare nanoparticles of gallium nitride (GaN) by reacting  $\text{Li}_3\text{N}$  and  $\text{GaCl}_3$  at  $280^\circ\text{C}$ .<sup>[4]</sup>

### *Packaging*

1, 6×1, 2 L in Sure/Seal™

100, 12×100 mL in Sure/Seal™

View [returnable container options](#).

