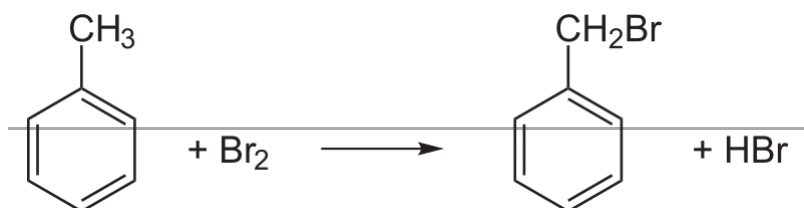


# Benzyl bromide

**Benzyl bromide** is an organic compound with the formula  $\text{C}_6\text{H}_5\text{CH}_2\text{Br}$ . The molecule consists of a benzene ring substituted with a bromomethyl group. It is a colorless liquid with lachrymatory properties. The compound is a reagent for introducing benzyl groups.<sup>[3][4]</sup>

## Synthesis and structure

Benzyl bromide can be synthesized by the bromination of toluene under conditions suitable for a free radical halogenation:



The structure has been examined by electron diffraction.<sup>[5]</sup>

## Applications

Benzyl bromide is used in organic synthesis for the introduction of the benzyl groups when the less expensive benzyl chloride is insufficiently reactive.<sup>[6]</sup> <sup>[7]</sup> Benzylations are often achieved in the presence of catalytic amounts of sodium iodide, which generates the more reactive benzyl iodide in situ.<sup>[3]</sup> In some cases, benzyl serves as protecting group for alcohols and carboxylic acids.<sup>[8]</sup>

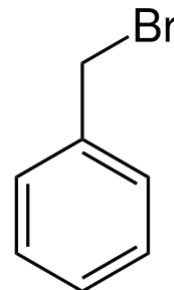
## Safety

Benzyl bromide is a strong lachrymator and is also intensely irritating to skin and mucous membranes. Because of these properties, it has been used in chemical warfare, both in combat and in training due to its irritating yet non-lethal nature.

## See also

- Benzyl chloride
- Benzyl fluoride

### Benzyl bromide<sup>[1]</sup>



#### Names

Preferred IUPAC name

(Bromomethyl)benzene

Other names

$\alpha$ -Bromotoluene

Benzyl bromide

#### Identifiers

CAS Number

100-39-0 ([https://com monchemistry.cas.org/detail?cas\\_rn=100-39-0](https://com monchemistry.cas.org/detail?cas_rn=100-39-0))<sup>✓</sup>

3D model (JSmol)

Interactive image (<https://chemapps.stolaf.edu/jmol/jmol.php?model=BrCc1ccccc1>)

Interactive image (<https://chemapps.stolaf.edu/jmol/jmol.php?model=c1ccc%28cc1%29CBr>)

ChEBI

CHEBI:59858 (<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=59858>)<sup>✓</sup>

ChEMBL


ChEMBL1085946 (<https://www.ebi.ac.uk/chembl/index.php/co>)

- [Benzyl iodide](#)

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	<a href="#">mpound/inspect/ChE MBL1085946</a> ✓
ChemSpider	13851576 ( <a href="https://www.chemspider.com/Chemical-Structure.13851576.html">https://www.chemspider.com/Chemical-Structure.13851576.html</a> ) ✓
ECHA InfoCard	100.002.589 ( <a href="https://echa.europa.eu/substance-information/-/substanceinfo/100.002.589">https://echa.europa.eu/substance-information/-/substanceinfo/100.002.589</a> )
IUPHAR/BPS	6294 ( <a href="http://www.guidetopharmacology.org/GRAC/LigandDisplayForward?tab=summary&amp;ligandId=6294">http://www.guidetopharmacology.org/GRAC/LigandDisplayForward?tab=summary&amp;ligandId=6294</a> )
PubChem CID	7498 ( <a href="https://pubchem.ncbi.nlm.nih.gov/compound/7498">https://pubchem.ncbi.nlm.nih.gov/compound/7498</a> )
UNII	XR75BS721D ( <a href="https://precision.fda.gov/uniisearch/srs/unii/XR75BS721D">https://precision.fda.gov/uniisearch/srs/unii/XR75BS721D</a> ) ✗
CompTox Dashboard (EPA)	DTXSID8024658 ( <a href="https://comptox.epa.gov/dashboard/chemical/details/DTXSID8024658">https://comptox.epa.gov/dashboard/chemical/details/DTXSID8024658</a> )
InChI	[show] InChI=1S/C7H7Br/c8-6-7-4-2-1-3-5-7/h1-5H,6H2 ✓ Key: AGEZXYOZHKGVCU-UHFFFAOYSA-N ✓
	InChI=1/C7H7Br/c8-6-7-4-2-1-3-5-7/h1-5H,6H2 Key: AGEZXYOZHKGVCU-UHFFFAOYAM
SMILES	[show] BrCc1ccccc1 c1ccc(cc1)CBr
<b>Properties</b>	
Chemical formula	C <sub>7</sub> H <sub>7</sub> Br

<u>Molar mass</u>	171.037 g·mol <sup>−1</sup>
<u>Appearance</u>	Colorless liquid
<u>Odor</u>	Sharp and pungent
<u>Density</u>	1.438 g/cm <sup>3</sup>
<u>Melting point</u>	−3.9 °C (25.0 °F; 269.2 K)
<u>Boiling point</u>	201 °C (394 °F; 474 K)
<u>Solubility</u>	organic solvents
<u>log <i>P</i></u>	2.92 <sup>[2]</sup>
<u>Refractive index (<i>n</i><sub>D</sub>)</u>	1.5752
<b>Hazards</b>	
<b>GHS labelling:</b>	
<u>Pictograms</u>	
<u>Flash point</u>	70 °C (158 °F; 343 K)
<p>Except where otherwise noted, data are given for materials in their <u>standard state</u> (at 25 °C [77 °F], 100 kPa).</p> <p><span>✗</span> <u>verify (what is <span>✓</span>✗ ?)</u></p> <p><u>Infobox references</u></p>	

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