

# Benzene, 1-azido-4-bromo-

<b>Other names:</b>	p-Bromophenyl azide 1-Azido-4-bromobenzene 4-Bromophenyl azide
<b>Inchi:</b>	InChI=1S/C6H4BrN3/c7-5-1-3-6(4-2-5)9-10-8/h1-4H
<b>InchiKey:</b>	WHSJSMSBFMDFHK-UHFFFAOYSA-N
<b>Formula:</b>	C6H4BrN3
<b>SMILES:</b>	[N-]=[N+]=Nc1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	198.02
<b>CAS:</b>	2101-88-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.29		Crippen Method
logp	3.391		Crippen Method
mcvol	110.480	ml/mol	McGowan Method
tf	293.00	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.00	K	1.30	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2101884&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2101884&amp;Units=SI</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tf:</b>	Normal melting (fusion) point

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