Benzene, 1-azido-4-bromo-

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2101884&Units=SI

Legend

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