

N-(Bromomethyl)phthalimide

Other names:	1H-Isoindole-1,3(2H)-dione, 2-(bromomethyl)-Phthalimide, N-(bromomethyl)-Phthalimidomethyl bromide
Inchi:	InChI=1S/C9H6BrNO2/c10-5-11-8(12)6-3-1-2-4-7(6)9(11)13/h1-4H,5H2
InchiKey:	UUSLLECLCKTJQF-UHFFFAOYSA-N
Formula:	C9H6BrNO2
SMILES:	O=C1c2ccccc2C(=O)N1CBr
Mol. weight [g/mol]:	240.05
CAS:	5332-26-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	1.635		Crippen Method
mcvol	133.670	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5332263&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/36-967-9/N-Bromomethyl-phthalimide.pdf>

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