

Pyridine, 3-bromo-, 1-oxide

Other names:	3-Bromo-pyridine 1-oxide
Inchi:	InChI=1S/C5H4BrNO/c6-5-2-1-3-7(8)4-5/h1-4H
InchiKey:	YUIBFWHMRBJHNV-UHFFFAOYSA-N
Formula:	C5H4BrNO
SMILES:	[O-][n+]1cccc(Br)c1
Mol. weight [g/mol]:	174.00
CAS:	2402-97-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	1.083		Crippen Method
mcvol	90.900	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=C2402973&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/42-865-5/Pyridine-3-bromo-1-oxide.pdf>

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