

2-Mercaptopyridine-N-oxide

Other names:	2-Pyridinethiol, 1-oxide
	2-Mercaptopyridine monoxide
	Omadine
	Pyridine-2-thiol-1-oxide
	pyridine-2-thiol N-oxide
Inchi:	InChI=1S/C5H5NOS/c7-6-4-2-1-3-5(6)8/h1-4,8H
InchiKey:	FGVVTMRZYROCTH-UHFFFAOYSA-N
Formula:	C5H5NOS
SMILES:	[O-][n+]1ccccc1S
Mol. weight [g/mol]:	127.16
CAS:	1121-31-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	0.609		Crippen Method
mcvol	89.750	ml/mol	McGowan Method

Sources

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=C1121319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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