

3-Methylquinoline-1-oxide

Inchi:	InChI=1S/C10H9NO/c1-8-6-9-4-2-3-5-10(9)11(12)7-8/h2-7H,1H3
InchiKey:	CBGUMTBCWWMBRV-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	<chem>Cc1cc2ccccc2[n+]([O-])c1</chem>
Mol. weight [g/mol]:	159.18
CAS:	1873-55-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	1.782		Crippen Method
mcvol	124.390	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=C1873558&Units=SI

Legend

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

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<https://www.chemeo.com/cid/13-903-4/3-Methylquinoline-1-oxide.pdf>

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