

Quinoline, 6-methoxy-, 1-oxide

Other names:	6-Methoxyquinoline 1-oxide 6-Methoxyquinoline-N-oxide
Inchi:	InChI=1S/C10H9NO2/c1-13-9-4-5-10-8(7-9)3-2-6-11(10)12/h2-7H,1H3
InchiKey:	BWEGRKPOJXNZSK-UHFFFAOYSA-N
Formula:	C10H9NO2
SMILES:	COc1ccc2c(ccc[n+] ₂ [O-])c1
Mol. weight [g/mol]:	175.18
CAS:	6563-13-9

Physical Properties

Property code	Value	Unit	Source
hsub	117.90 ± 1.00	kJ/mol	NIST Webbook
log10ws	-4.92		Crippen Method
logp	1.482		Crippen Method
mcvol	130.260	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6563139&Units=SI
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

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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