

5-Bromo-6-methoxy-8-nitroquinoline

Inchi:	InChI=1S/C10H7BrN2O3/c1-16-8-5-7(13(14)15)10-6(9(8)11)3-2-4-12-10/h2-5H,1H3
InchiKey:	SDMIYMJTQNOZRV-UHFFFAOYSA-N
Formula:	C10H7BrN2O3
SMILES:	COc1cc([N+](=O)[O-])c2ncccc2c1Br
Mol. weight [g/mol]:	283.08
CAS:	5347-15-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Crippen Method
logp	2.914		Crippen Method
mcvol	159.310	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=C5347159&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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