

5-Methoxy-8-nitro-quinoline

Inchi:	InChI=1S/C10H8N2O3/c1-15-9-5-4-8(12(13)14)10-7(9)3-2-6-11-10/h2-6H,1H3
InchiKey:	RWFYICPQQAJGAK-UHFFFAOYSA-N
Formula:	C10H8N2O3
SMILES:	COc1ccc([N+](=O)[O-])c2ncccc12
Mol. weight [g/mol]:	204.18
CAS:	36020-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.152		Crippen Method
mcvol	141.810	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=C36020538&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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