

Quinoline, 6-methoxy-8-nitro-

Other names:	6-Methoxy-8-nitroquinoline 8-Nitro-6-methoxyquinoline methyl 8-nitro-6-quinolyl ether
Inchi:	InChI=1S/C10H8N2O3/c1-15-8-5-7-3-2-4-11-10(7)9(6-8)12(13)14/h2-6H,1H3
InchiKey:	MIMUSZHMZBJBPO-UHFFFAOYSA-N
Formula:	C10H8N2O3
SMILES:	COc1cc([N+](=O)[O-])c2cccc2c1
Mol. weight [g/mol]:	204.18
CAS:	85-81-4

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/46-912-8/Quinoline-6-methoxy-8-nitro.pdf>

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