

2-(Dimethylamino)-5-nitropyridine

Other names:	N,N-dimethyl-5-nitropyridin-2-amine
Inchi:	InChI=1S/C7H9N3O2/c1-9(2)7-4-3-6(5-8-7)10(11)12/h3-5H,1-2H3
InchiKey:	UCAOGXRUIJFKQAP-UHFFFAOYSA-N
Formula:	C7H9N3O2
SMILES:	CN(C)c1ccc([N+](=O)[O-])cn1
Mol. weight [g/mol]:	167.17
CAS:	2554-75-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.056		Crippen Method
mcvol	123.110	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=C2554758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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