

2-Methyl-5-nitrobenzimidazole

Other names:	1H-Benzimidazole, 2-methyl-5-nitro-Benzimidazole, 2-methyl-5-nitro-Benzimidazole, 2-methyl-5(or 6)-nitro-2-Methyl-6-nitrobenzimidazole 5-Nitro-2-methylbenzimidazole 2-Methyl-6-nitro-1H-benzoimidazole 2-methyl-5-nitro-1H-benzimidazole
Inchi:	InChI=1S/C8H7N3O2/c1-5-9-7-3-2-6(11(12)13)4-8(7)10-5/h2-4H,1H3,(H,9,10)
InchiKey:	RKRXTVLCZDPERO-UHFFFAOYSA-N
Formula:	C8H7N3O2
SMILES:	<chem>Cc1nc2cc([N+](=O)[O-])ccc2[nH]1</chem>
Mol. weight [g/mol]:	177.16
CAS:	1792-40-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	1.298		Crippen Method
mvol	122.040	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=C1792401&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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