

4-nitroimidazole

Other names:	4(5)-nitroimidazole 4-nitro-1H-imidazole 5-nitro-1H-imidazole 5-nitroimidazole
Inchi:	InChI=1S/C3H3N3O2/c7-6(8)3-1-4-2-5-3/h1-2H,(H,4,5)
InchiKey:	VYDWQPKRHOGLPA-UHFFFAOYSA-N
Formula:	C3H3N3O2
SMILES:	O=[N+](O)c1cnc[nH]1
Mol. weight [g/mol]:	113.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.11		Crippen Method
logp	-0.164		Crippen Method
mcvol	71.050	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	122.90	kJ/mol	298.15	Calorimetric and computational studies for three nitroimidazole isomers

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Calorimetric and computational studies for three nitroimidazole isomers:	https://www.doi.org/10.1016/j.jct.2016.10.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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