1H-Imidazole, 1-methyl-5-nitro-

Other names:	Imidazole, 1-methyl-5-nitro-
	1-Methyl-5-nitroimidazole
	1-Methyl-5-nitro-1H-imidazole
Inchi:	InChI=1S/C4H5N3O2/c1-6-3-5-2-4(6)7(8)9/h2-3H,1H3
InchiKey:	JLZXSFPSJJMRIX-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	Cn1cncc1[N+](=O)[O-]
Mol. weight [g/mol]:	127.10
CAS:	3034-42-2

Physical Properties

Property code	Value	Unit	Source
affp	895.30	kJ/mol	NIST Webbook
basg	863.50	kJ/mol	NIST Webbook
log10ws	-3.18		Crippen Method
logp	0.328		Crippen Method
mcvol	85.140	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3034422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume