5-Chloro-1-methyl-4-nitroimidazole

Other names:	1-methyl-4-nitro-5-chloroimidazole
	5-chloro-1-methyl-4-nitro-1H-imidazole
	A(S50154-9)
	Imidazole, 5-chloro-1-methyl-4-nitro-
Inchi:	InChI=1S/C4H4ClN3O2/c1-7-2-6-4(3(7)5)8(9)10/h2H,1H3
InchiKey:	OSJUNMSWBBOTQU-UHFFFAOYSA-N
Formula:	C4H4ClN3O2
SMILES:	Cn1cnc([N+](=O)[O-])c1Cl
Mol. weight [g/mol]:	161.55

Physical Properties

Property code	Value	Unit	Source
logp	0.982		Crippen Method
mcvol	97.380	ml/mol	McGowan Method
tf	421.35	K	Thermodynamic modelling for solubility of 5-chloro-1-methyl-4-nitroimidazole in eleven organic solvents from T = (283.15 to 318.15) K

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermodynamic modelling for solubility of 5-chloro-1-methyl-4-nitroimidazole in eleven organic solvents from T = (283.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2016.10.006
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4897250&Units=SI

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point