Imidazole, 4-methyl-5-nitro-

Other names:	Imidazole, 4-methyl-5-nitro-
	4-Methyl-5-nitroimidazole
	5-Methyl-4-nitroimidazole
	Imidazole, 5-methyl-4-nitro-
	4-Methyl-5-nitro-1H-imidazole
	Imidazole, 4(or 5)-methyl-5(or 4)-nitro-
Inchi:	InChI=1S/C4H5N3O2/c1-3-4(7(8)9)6-2-5-3/h2H,1H3,(H,5,6)
InchiKey:	WSYOWIMKNNMEMZ-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	Cc1nc[nH]c1[N+](=O)[O-]
Mol. weight [g/mol]:	127.10

Physical Properties

Property code	Value	Unit	Source
logp	0.144		Crippen Method
mcvol	85.140	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14003668&Units=SI
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):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume