1H-BENZIMIDAZOLE, 2-METHYL-5-NITRO-

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:	Cc1nc2cc([N+](=O)[O-])ccc2[nH]1
Mol. weight [g/mol]:	177.16

Physical Properties

Property code	Value	Unit	Source
hf	117.25	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	1.298		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
tb	592.09	K	Cheméo Relay (1.0)
tf	560.74	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1792401&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

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point