Benzothiazole, 2-methyl-6-nitro-

Other names: 2-Methyl-6-nitrobenzothiazole
Inchi: InChI=1S/C8H6N2O2S/c1-5-9-7-3-2-6(10(11)12)4-8(7)13-5/h2-4H,1H3
InchiKey: YAQKYKGFPQPPQE-UHFFFAOYSA-N
Formula: C8H6N2O2S
SMILES: Cc1nc2ccc([N+](=O)[O-])cc2s1
Mol. weight [g/mol]: 194.21
CAS: 2941-63-1

Physical Properties

Property code	Value	Unit	Source
ie	9.15	eV	NIST Webbook
log10ws	-3.93		Crippen Method
logp	2.513		Crippen Method
mcvol	128.410	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2941631&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume