

Isothiazole, 4-nitro-

Other names:	4-Nitroisothiazole
Inchi:	InChI=1S/C3H2N2O2S/c6-5(7)3-1-4-8-2-3/h1-2H
InchiKey:	FNXPAYVHLSTHQY-UHFFFAOYSA-N
Formula:	C3H2N2O2S
SMILES:	O=[N+](O-)c1cnsc1
Mol. weight [g/mol]:	130.12
CAS:	931-07-7

Physical Properties

Property code	Value	Unit	Source
ie	10.45	eV	NIST Webbook
log10ws	-1.65		Crippen Method
logp	1.051		Crippen Method
mcvol	77.420	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C931077&Units=SI

Legend

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

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<https://www.chemeo.com/cid/16-896-0/Isothiazole-4-nitro.pdf>

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