Isothiazole

Inchi: InChI=1S/C3H3NS/c1-2-4-5-3-1/h1-3H
InchiKey: ZLTPDFXIESTBQG-UHFFFAOYSA-N
Formula: C3H3NS
SMILES: c1cnsc1
Mol. weight [g/mol]: 85.13
CAS: 288-16-4

Physical Properties

Property code	Value	Unit	Source
ie	9.80	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
ie	9.62	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	1.143		Crippen Method
mcvol	60.000	ml/mol	McGowan Method

Sources

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=C288164&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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