

Isothiocyanic acid

Inchi: InChI=1S/CNS/c2-1-3/q-1
InchiKey: ZBKFYXZXZJPWNQ-UHFFFAOYSA-N
Formula: CHNS
SMILES: [N-]=C=S
Mol. weight [g/mol]: 59.09
CAS: 3129-90-6

Physical Properties

Property code	Value	Unit	Source
ie	9.92	eV	NIST Webbook
ie	9.92	eV	NIST Webbook
ie	10.10 ± 0.10	eV	NIST Webbook
ie	9.94 ± 0.02	eV	NIST Webbook
log10ws	-3.25		Crippen Method
logp	0.659		Crippen Method
mcvol	40.530	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=C3129906&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/29-758-9/Isothiocyanic-acid.pdf>

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