

1-Isothiocyanatoethylene

Inchi: InChI=1S/C3H3NS/c1-2-4-3-5/h2H,1H2
InchiKey: VJCLZQUHGQSTMZ-UHFFFAOYSA-N
Formula: C3H3NS
SMILES: C=CN=C=S
Mol. weight [g/mol]: 85.13
CAS: 1520-22-5

Physical Properties

Property code	Value	Unit	Source
hf	304.25	kJ/mol	Joback Method
hvap	32.04	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.233		Crippen Method
mvol	66.560	ml/mol	McGowan Method
pc	4809.16	kPa	Joback Method
tb	410.67	K	Joback Method
tc	639.84	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1520225&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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