

Methyl 2-isothiocyanatoacetate

Inchi: InChI=1S/C4H5NO2S/c1-7-4(6)2-5-3-8/h2H2,1H3
InchiKey: GOWGDPFDGIPFIK-UHFFFAOYSA-N
Formula: C4H5NO2S
SMILES: COC(=O)CN=C=S
Mol. weight [g/mol]: 131.15
CAS: 21055-37-8

Physical Properties

Property code	Value	Unit	Source
hf	-86.62	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.262		Crippen Method
mcvol	92.390	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	513.16	K	Joback Method
tc	742.64	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21055378&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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