

3-Methoxypropyl isothiocyanate

Inchi: InChI=1S/C5H9NOS/c1-7-4-2-3-6-5-8/h2-4H2,1H3
InchiKey: UKVFWFDXYBLOLU-UHFFFAOYSA-N
Formula: C5H9NOS
SMILES: COCCCN=C=S
Mol. weight [g/mol]: 131.20
CAS: 17702-11-3

Physical Properties

Property code	Value	Unit	Source
hf	5.32	kJ/mol	Joback Method
hvap	39.57	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	1.126		Crippen Method
mvol	104.910	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	482.17	K	Joback Method
tc	697.94	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C17702113&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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