

Ethane, 1-isothiocyanato-2-methoxy-

Other names:	2-methoxyethyl isothiocyanate
Inchi:	InChI=1S/C4H7NOS/c1-6-3-2-5-4-7/h2-3H2,1H3
InchiKey:	HTSAVXAFEVUJQE-UHFFFAOYSA-N
Formula:	C4H7NOS
SMILES:	COCCN=C=S
Mol. weight [g/mol]:	117.17
CAS:	38663-85-3

Physical Properties

Property code	Value	Unit	Source
hf	25.96	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.736		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	459.29	K	Joback Method
tc	678.34	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38663853&Units=SI

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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