Ethoxycarbonyl isothiocyanate

Other names:	Carbethoxy isothiocyanate Carbon(isothiocyanatidic) acid, ethyl ester ethyl isothiocyanatoformate
Inchi:	InChI=1S/C4H5NO2S/c1-2-7-4(6)5-3-8/h2H2,1H3
InchiKey:	BDTDECDAHYOJRO-UHFFFAOYSA-N
Formula:	C4H5NO2S
SMILES:	CCOC(=O)N=C=S
Mol. weight [g/mol]:	131.15
CAS:	16182-04-0

Physical Properties

Property code	Value	Unit	Source
hf	-86.62	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.246		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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C16182040&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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