Ethyl 4-isothiocyanatobutyrate

Other names:	Ethyl 4-isothiocyanatobutanoate
	4-Isothiocyanato-butyric acid ethyl ester
	Butyric acid, 4-isothiocyanato-, ethyl ester
Inchi:	InChI=1S/C7H11NO2S/c1-2-10-7(9)4-3-5-8-6-11/h2-5H2,1H3
InchiKey:	FAGABVVHWPYGBK-UHFFFAOYSA-N
Formula:	C7H11NO2S
SMILES:	CCOC(=O)CCCN=C=S
Mol. weight [g/mol]:	173.23
CAS:	17126-65-7

Physical Properties

Property code	Value	Unit	Source
hf	-148.54	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.433		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1346.80		NIST Webbook
rinpol	1346.80		NIST Webbook
tb	581.80	K	Joback Method
tc	799.17	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=C17126657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:
https://www.chemeo.com/cid/56-608-5/Ethyl-4-isothiocyanatobutyrate.pdf
Generated by Cheméo on 2024-04-29 12:05:42.09293551 +0000 UTC m=+16681591.013512826.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.