2-Isothiocyanato-butyric acid ethyl ester

Inchi: InChI=1S/C7H11NO3/c1-3-6(8-5-9)7(10)11-4-2/h6H,3-4H2,1-2H3
InchiKey: UTFCRCGRAVHBRB-UHFFFAOYSA-N
Formula: C7H11NO3
SMILES: CCOC(=O)C(CC)N=C=O
Mol. weight [g/mol]: 157.17

Physical Properties

Property code	Value	Unit	Source
hf	-443.30	kJ/mol	Joback Method
hvap	49.48	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	0.664		Crippen Method
mcvol	124.180	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	1217.60		NIST Webbook
tb	502.08	K	Joback Method
tc	692.47	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R319974&Units=SI
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

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