Ethyl 3-isothiocyanatobutyrate

Inchi: InChI=1S/C7H11NO2S/c1-3-10-7(9)4-6(2)8-5-11/h6H,3-4H2,1-2H3
InchiKey: BJPWLYQGLIRJLZ-UHFFFAOYSA-N
Formula: C7H11NO2S
SMILES: CCOC(=O)CC(C)N=C=S
Mol. weight [g/mol]: 173.23
CAS: 206750-29-0

Physical Properties

Property code	Value	Unit	Source
hf	-153.82	kJ/mol	Joback Method
hvap	50.38	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.431		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	581.36	K	Joback Method
tc	803.43	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=C206750290&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