Ethyl 2-isocyanato-4-methylthiobutyrate

Inchi: InChI=1S/C8H13NO3S/c1-3-12-8(11)7(9-6-10)4-5-13-2/h7H,3-5H2,1-2H3
InchiKey: IWXRXGRHXXLVHJ-UHFFFAOYSA-N
Formula: C8H13NO3S
SMILES: CCOC(=O)C(CCSC)N=C=O
Mol. weight [g/mol]: 203.26
CAS: 64505-12-0

Physical Properties

Property code	Value	Unit	Source
hf	-422.07	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	1.007		Crippen Method
mcvol	154.620	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	593.74	K	Joback Method
tc	799.36	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=C64505120&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