

# 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/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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