

# Methyl 2-isothiocyanato-3-methylbutyrate

**Inchi:** InChI=1S/C7H11NO2S/c1-5(2)6(8-4-11)7(9)10-3/h5-6H,1-3H3  
**InchiKey:** MFTMQIVHQZBFTC-UHFFFAOYSA-N  
**Formula:** C7H11NO2S  
**SMILES:** COC(=O)C(N=C=S)C(C)C  
**Mol. weight [g/mol]:** 173.23  
**CAS:** 114877-91-7

## Physical Properties

Property code	Value	Unit	Source
hf	-159.10	kJ/mol	Joback Method
hvap	50.00	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.287		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	580.92	K	Joback Method
tc	807.86	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C114877917&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**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)

## 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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