

# 2-Isothiocyanato-3-methylbutyric acid ethyl ester

**Inchi:** InChI=1S/C8H13NO2S/c1-4-11-8(10)7(6(2)3)9-5-12/h6-7H,4H2,1-3H3  
**InchiKey:** MWCPMVGNNCNCZPM-UHFFFAOYSA-N  
**Formula:** C8H13NO2S  
**SMILES:** CCOC(=O)C(N=C=S)C(C)C  
**Mol. weight [g/mol]:** 187.26

## Physical Properties

Property code	Value	Unit	Source
hf	-179.74	kJ/mol	Joback Method
hvap	52.22	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.677		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1271.00		NIST Webbook
tb	603.80	K	Joback Method
tc	826.50	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177205&Units=SI>  
**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)

## 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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