

# 2-Isothiocyanato-3-(methylthio)propionic acid ethyl ester

**Inchi:** InChI=1S/C7H11NO2S2/c1-3-10-7(9)6(4-12-2)8-5-11/h6H,3-4H2,1-2H3  
**InchiKey:** LNIKMLXQQRUFGX-UHFFFAOYSA-N  
**Formula:** C7H11NO2S2  
**SMILES:** CCOC(=O)C(CSC)N=C=S  
**Mol. weight [g/mol]:** 205.30

## Physical Properties

Property code	Value	Unit	Source
hf	-111.95	kJ/mol	Joback Method
hvap	57.20	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.384		Crippen Method
mcvol	151.010	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1609.20		NIST Webbook
tb	650.14	K	Joback Method
tc	889.72	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](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=R177225&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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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