

# 6-Isothiocyanato-hexanoic acid ethyl ester

**Inchi:** InChI=1S/C9H15NO2S/c1-2-12-9(11)6-4-3-5-7-10-8-13/h2-7H2,1H3  
**InchiKey:** KYKPHLIHLIZMOO-UHFFFAOYSA-N  
**Formula:** C9H15NO2S  
**SMILES:** CCOC(=O)CCCCCN=C=S  
**Mol. weight [g/mol]:** 201.29

## Physical Properties

Property code	Value	Unit	Source
hf	-189.82	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.213		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1574.30		NIST Webbook
rinpol	1574.30		NIST Webbook
tb	627.56	K	Joback Method
tc	837.75	K	Joback Method

## Sources

**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=R177334&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)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	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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