

# Ethoxycarbonyl isothiocyanate

<b>Other names:</b>	Carbethoxy isothiocyanate Carbon(isothiocyanatidic) acid, ethyl ester ethyl isothiocyanatoformate
<b>Inchi:</b>	InChI=1S/C4H5NO2S/c1-2-7-4(6)5-3-8/h2H2,1H3
<b>InchiKey:</b>	BDTDECDAHYOJRO-UHFFFAOYSA-N
<b>Formula:</b>	C4H5NO2S
<b>SMILES:</b>	CCOC(=O)N=C=S
<b>Mol. weight [g/mol]:</b>	131.15
<b>CAS:</b>	16182-04-0

## Physical Properties

Property code	Value	Unit	Source
hf	-86.62	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.246		Crippen Method
mcvol	92.390	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	513.16	K	Joback Method
tc	742.64	K	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16182040&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16182040&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</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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