

# 3-Ethoxycarbonylphenyl isothiocyanate

<b>Inchi:</b>	InChI=1S/C10H9NO2S/c1-2-13-10(12)8-4-3-5-9(6-8)11-7-14/h3-6H,2H2,1H3
<b>InchiKey:</b>	MCHONYMFRSKTLR-UHFFFAOYSA-N
<b>Formula:</b>	C10H9NO2S
<b>SMILES:</b>	CCOC(=O)c1cccc(N=C=S)c1
<b>Mol. weight [g/mol]:</b>	207.25
<b>CAS:</b>	3137-84-6

## Physical Properties

Property code	Value	Unit	Source
hf	14.60	kJ/mol	Joback Method
hvap	60.39	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.598		Crippen Method
mcvol	153.170	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	682.10	K	Joback Method
tc	933.38	K	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C3137846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3137846&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>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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