

# Benzene, 1-ethoxy-4-isothiocyanato-

<b>Other names:</b>	Phenylisothiocyanate, 4-ethoxy p-ethoxyphenyl isothiocyanate
<b>Inchi:</b>	InChI=1S/C9H9NOS/c1-2-11-9-5-3-8(4-6-9)10-7-12/h3-6H,2H2,1H3
<b>InchiKey:</b>	REEKOMRZYJXXNR-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NOS
<b>SMILES:</b>	CCOc1ccc(N=C=S)cc1
<b>Mol. weight [g/mol]:</b>	179.24
<b>CAS:</b>	3460-49-9

## Physical Properties

Property code	Value	Unit	Source
hf	147.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.820		Crippen Method
mcvol	137.510	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	605.35	K	Joback Method
tc	856.17	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3460499&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3460499&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

## Legend

hf: 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>	Log10 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>p<sub>c</sub>:</b>	Critical Pressure
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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