

# 2-Methoxybenzyl isothiocyanate

**Inchi:** InChI=1S/C9H9NOS/c1-11-9-5-3-2-4-8(9)6-10-7-12/h2-5H,6H2,1H3  
**InchiKey:** HUYOVUYNRGOCLZ-UHFFFAOYSA-N  
**Formula:** C9H9NOS  
**SMILES:** COc1ccccc1CN=C=S  
**Mol. weight [g/mol]:** 179.24  
**CAS:** 17608-09-2

## Physical Properties

Property code	Value	Unit	Source
hf	147.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.298		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

**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=C17608092&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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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