

# 3,5-Dimethoxyphenyl isothiocyanate

**Inchi:** InChI=1S/C9H9NO2S/c1-11-8-3-7(10-6-13)4-9(5-8)12-2/h3-5H,1-2H3  
**InchiKey:** FKUHOOASBHTEQY-UHFFFAOYSA-N  
**Formula:** C9H9NO2S  
**SMILES:** COc1cc(N=C=S)cc(OC)c1  
**Mol. weight [g/mol]:** 195.24  
**CAS:** 104968-58-3

## Physical Properties

Property code	Value	Unit	Source
hf	4.13	kJ/mol	Joback Method
hvap	54.49	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.438		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	632.75	K	Joback Method
tc	880.39	K	Joback Method

## Sources

**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)  
**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=C104968583&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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