

# 3,4-Dimethylbenzyl isothiocyanate

**Inchi:** InChI=1S/C10H11NS/c1-8-3-4-10(5-9(8)2)6-11-7-12/h3-5H,6H2,1-2H3  
**InchiKey:** BNOGRVSYSGZCDC-UHFFFAOYSA-N  
**Formula:** C10H11NS  
**SMILES:** Cc1ccc(CN=C=S)cc1C  
**Mol. weight [g/mol]:** 177.27  
**CAS:** 206559-59-3

## Physical Properties

Property code	Value	Unit	Source
hf	247.93	kJ/mol	Joback Method
hvap	51.89	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.906		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
tb	610.79	K	Joback Method
tc	861.13	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C206559593&Units=SI>  
**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)

## 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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