

# 2,4-Dichlorobenzyl isothiocyanate

**Inchi:** InChI=1S/C8H5Cl2NS/c9-7-2-1-6(4-11-5-12)8(10)3-7/h1-3H,4H2  
**InchiKey:** JZHPXEMPVDMDFB-UHFFFAOYSA-N  
**Formula:** C8H5Cl2NS  
**SMILES:** S=C=NCc1ccc(Cl)cc1Cl  
**Mol. weight [g/mol]:** 218.10  
**CAS:** 18967-41-4

## Physical Properties

Property code	Value	Unit	Source
hf	257.73	kJ/mol	Joback Method
hvap	56.21	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.596		Crippen Method
mcvol	142.030	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	639.89	K	Joback Method
tc	908.27	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=C18967414&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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