

# 2,4,6-Trimethylphenyl isothiocyanate

**Inchi:** InChI=1S/C10H11NS/c1-7-4-8(2)10(11-6-12)9(3)5-7/h4-5H,1-3H3  
**InchiKey:** KKYMYPLVBCVDPL-UHFFFAOYSA-N  
**Formula:** C10H11NS  
**SMILES:** Cc1cc(C)c(N=C=S)c(C)c1  
**Mol. weight [g/mol]:** 177.27  
**CAS:** 6095-82-5

## Physical Properties

Property code	Value	Unit	Source
hf	236.46	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.346		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	615.77	K	Joback Method
tc	867.11	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6095825&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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