

# 3-Methylthiophenyl isocyanate

**Inchi:** InChI=1S/C8H7NOS/c1-11-8-4-2-3-7(5-8)9-6-10/h2-5H,1H3  
**InchiKey:** BKJABLMNBSVKCV-UHFFFAOYSA-N  
**Formula:** C8H7NOS  
**SMILES:** CSc1cccc(N=C=O)c1  
**Mol. weight [g/mol]:** 165.21  
**CAS:** 28479-19-8

## Physical Properties

Property code	Value	Unit	Source
hf	53.07	kJ/mol	Joback Method
hvap	52.69	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	2.376		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	549.55	K	Joback Method
tc	793.68	K	Joback Method

## Sources

**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=C28479198&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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