

# 4-Methylbenzoyl isothiocyanate

**Inchi:** InChI=1S/C9H7NOS/c1-7-2-4-8(5-3-7)9(11)10-6-12/h2-5H,1H3  
**InchiKey:** RZCAJUGXEPHWJY-UHFFFAOYSA-N  
**Formula:** C9H7NOS  
**SMILES:** Cc1ccc(C(=O)N=C=S)cc1  
**Mol. weight [g/mol]:** 177.22  
**CAS:** 16794-68-6

## Physical Properties

Property code	Value	Unit	Source
hf	167.46	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.238		Crippen Method
mcvol	133.210	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	636.80	K	Joback Method
tc	898.72	K	Joback Method

## Sources

**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=C16794686&Units=SI>  
**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)

## 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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