

# 3-Nitrobenzoyl isothiocyanate

**Inchi:** InChI=1S/C8H4N2O3S/c11-8(9-5-14)6-2-1-3-7(4-6)10(12)13/h1-4H  
**InchiKey:** BPIGGCBDZBMLCI-UHFFFAOYSA-N  
**Formula:** C8H4N2O3S  
**SMILES:** O=C(N=C=S)c1cccc([N+](=O)[O-])c1  
**Mol. weight [g/mol]:** 208.19  
**CAS:** 78225-78-2

## Physical Properties

Property code	Value	Unit	Source
hf	177.34	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.838		Crippen Method
mcvol	136.540	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	765.76	K	Joback Method
tc	1053.07	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=C78225782&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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