

# 4-Ethylphenyl isothiocyanate

**Inchi:** InChI=1S/C9H9NS/c1-2-8-3-5-9(6-4-8)10-7-11/h3-6H,2H2,1H3  
**InchiKey:** XXLWCGRHJFEMQH-UHFFFAOYSA-N  
**Formula:** C9H9NS  
**SMILES:** CCc1ccc(N=C=S)cc1  
**Mol. weight [g/mol]:** 163.24  
**CAS:** 18856-63-8

## Physical Properties

Property code	Value	Unit	Source
hf	280.04	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.983		Crippen Method
mcvol	131.640	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	582.93	K	Joback Method
tc	837.99	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=C18856638&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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