

# (7-Isothiocyanatoheptyl)(methyl)sulfane

**Inchi:** InChI=1S/C9H17NS2/c1-12-8-6-4-2-3-5-7-10-9-11/h2-8H2,1H3  
**InchiKey:** LDIRGNDMTOGVRB-UHFFFAOYSA-N  
**Formula:** C9H17NS2  
**SMILES:** CSCCCCCCN=C=S  
**Mol. weight [g/mol]:** 203.37  
**CAS:** 4430-38-0

## Physical Properties

Property code	Value	Unit	Source
hf	96.85	kJ/mol	Joback Method
hvap	52.89	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.403		Crippen Method
mcvol	171.750	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1773.20		NIST Webbook
rinpol	1773.20		NIST Webbook
tb	620.05	K	Joback Method
tc	842.42	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4430380&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)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>r<sub>inpol</sub>:</b>	Non-polar retention indices
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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