

# 2-Pentane isothiocyanate

**Inchi:** InChI=1S/C6H11NS/c1-3-4-6(2)7-5-8/h6H,3-4H2,1-2H3  
**InchiKey:** SQBOSXLLKLBNSH-UHFFFAOYSA-N  
**Formula:** C6H11NS  
**SMILES:** CCCC(C)N=C=S  
**Mol. weight [g/mol]:** 129.22  
**CAS:** 201224-94-4

## Physical Properties

Property code	Value	Unit	Source
hf	111.62	kJ/mol	Joback Method
hvap	39.00	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.278		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	482.19	K	Joback Method
tc	701.74	K	Joback Method

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C201224944&Units=SI>

## 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

Latest version available from:

<https://www.chemeo.com/cid/41-574-9/2-Pentane-isothiocyanate.pdf>

Generated by Cheméo on 2024-04-27 02:30:48.910400204 +0000 UTC m=+16474297.830977520.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.