

# 1,4-Butane diisothiocyanate

**Inchi:** InChI=1S/C6H8N2S2/c9-5-7-3-1-2-4-8-6-10/h1-4H2  
**InchiKey:** RRSISCMPUAGVJN-UHFFFAOYSA-N  
**Formula:** C6H8N2S2  
**SMILES:** S=C=NCCCCN=C=S  
**Mol. weight [g/mol]:** 172.27  
**CAS:** 4430-51-7

## Physical Properties

Property code	Value	Unit	Source
hf	400.97	kJ/mol	Joback Method
hvap	49.83	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.972		Crippen Method
mcvol	130.860	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	628.58	K	Joback Method
tc	885.40	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**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=C4430517&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/14-215-7/1-4-Butane-diisothiocyanate.pdf>

Generated by Cheméo on 2024-05-03 00:00:59.356771657 +0000 UTC m=+16983708.277348967.

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