

# 1-Isothiocyanato-7-(methylsulfinyl)heptane

<b>Inchi:</b>	InChI=1S/C9H17NOS2/c1-13(11)8-6-4-2-3-5-7-10-9-12/h2-8H2,1H3
<b>InchiKey:</b>	OGYHCBGORZWBPH-UHFFFAOYSA-N
<b>Formula:</b>	C9H17NOS2
<b>SMILES:</b>	CS(=O)CCCCCCN=C=S
<b>Mol. weight [g/mol]:</b>	219.37
<b>CAS:</b>	129244-98-0

## Physical Properties

Property code	Value	Unit	Source
hf	-150.76	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.418		Crippen Method
mcpvol	177.620	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	609.55	K	Joback Method
tc	819.33	K	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C129244980&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C129244980&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## 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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