

# Hexane, 1-isothiocyanato-

<b>Other names:</b>	Isothiocyanic acid, hexyl ester Hexyl isothiocyanate n-Hexyl isothiocyanate 1-hexyl isothiocyanate
<b>Inchi:</b>	InChI=1S/C7H13NS/c1-2-3-4-5-6-8-7-9/h2-6H2,1H3
<b>InchiKey:</b>	WXYAXKKXIGHXDS-UHFFFAOYSA-N
<b>Formula:</b>	C7H13NS
<b>SMILES:</b>	CCCCCN=C=S
<b>Mol. weight [g/mol]:</b>	143.25
<b>CAS:</b>	4404-45-9

## Physical Properties

Property code	Value	Unit	Source
hf	96.26	kJ/mol	Joback Method
hvap	41.62	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.670		Crippen Method
mvol	127.220	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1199.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1181.20		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1581.00		NIST Webbook
tb	505.51	K	Joback Method
tc	716.71	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4404459&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4404459&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>
<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>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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