

# Methoxymethyl isothiocyanate

<b>Other names:</b>	Methane, isothiocyanatomethoxy-
<b>Inchi:</b>	InChI=1S/C3H5NOS/c1-5-2-4-3-6/h2H2,1H3
<b>InchiKey:</b>	SWHVODLGSMJMND-UHFFFAOYSA-N
<b>Formula:</b>	C3H5NOS
<b>SMILES:</b>	COCN=C=S
<b>Mol. weight [g/mol]:</b>	103.14
<b>CAS:</b>	19900-84-6

## Physical Properties

Property code	Value	Unit	Source
hf	46.60	kJ/mol	Joback Method
hvap	35.12	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.693		Crippen Method
mcvol	76.730	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
tb	436.41	K	Joback Method
tc	658.64	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=C19900846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19900846&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

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</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>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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