

# N-Allyl O-methyl thiocarbamate

<b>Inchi:</b>	InChI=1S/C5H9NOS/c1-3-4-6-5(8)7-2/h3H,1,4H2,2H3,(H,6,8)
<b>InchiKey:</b>	KFQCYQPZTRDLBX-UHFFFAOYSA-N
<b>Formula:</b>	C5H9NOS
<b>SMILES:</b>	C=CCNC(=S)OC
<b>Mol. weight [g/mol]:</b>	131.20
<b>CAS:</b>	41596-55-8

## Physical Properties

Property code	Value	Unit	Source
gf	180.51	kJ/mol	Joback Method
hf	46.65	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	41.63	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.693		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1115.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1948.00		NIST Webbook
tb	453.11	K	Joback Method
tc	656.21	K	Joback Method
tf	253.51	K	Joback Method
vc	0.386	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.14	J/molxK	453.11	Joback Method
cpg	209.25	J/molxK	486.96	Joback Method
cpg	217.83	J/molxK	520.81	Joback Method
cpg	225.90	J/molxK	554.66	Joback Method
cpg	233.49	J/molxK	588.51	Joback Method
cpg	240.64	J/molxK	622.36	Joback Method

## Sources

<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>
<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=C41596558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41596558&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion 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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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