

# N-Ethyl O-methyl thiocarbamate

<b>Inchi:</b>	InChI=1S/C4H9NOS/c1-3-5-4(7)6-2/h3H2,1-2H3,(H,5,7)
<b>InchiKey:</b>	ZYOAATWGQPZZFV-UHFFFAOYSA-N
<b>Formula:</b>	C4H9NOS
<b>SMILES:</b>	CCNC(=S)OC
<b>Mol. weight [g/mol]:</b>	119.19
<b>CAS:</b>	65351-53-3

## Physical Properties

Property code	Value	Unit	Source
gf	84.25	kJ/mol	Joback Method
hf	-58.14	kJ/mol	Joback Method
hfus	17.01	kJ/mol	Joback Method
hvap	40.07	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.527		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
rinpol	1046.00		NIST Webbook
tb	433.55	K	Joback Method
tc	634.57	K	Joback Method
tf	244.00	K	Joback Method
vc	0.348	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.16	J/molxK	433.55	Joback Method
cpg	186.72	J/molxK	467.05	Joback Method
cpg	194.82	J/molxK	500.56	Joback Method
cpg	202.49	J/molxK	534.06	Joback Method
cpg	209.74	J/molxK	567.56	Joback Method
cpg	216.59	J/molxK	601.07	Joback Method
cpg	223.08	J/molxK	634.57	Joback Method

# Sources

<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=C65351533&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C65351533&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>rinpola:</b>	Non-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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