

# Methyl N-chloroacetylcarbamate

<b>Inchi:</b>	InChI=1S/C4H6ClNO3/c1-9-4(8)6-3(7)2-5/h2H2,1H3,(H,6,7,8)
<b>InchiKey:</b>	SYWSERLZKPGKDI-UHFFFAOYSA-N
<b>Formula:</b>	C4H6ClNO3
<b>SMILES:</b>	COC(=O)NC(=O)CCl
<b>Mol. weight [g/mol]:</b>	151.55
<b>CAS:</b>	13558-70-8

## Physical Properties

Property code	Value	Unit	Source
gf	-302.58	kJ/mol	Joback Method
hf	-445.54	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	51.22	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.108		Crippen Method
mcvol	98.450	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	508.68	K	Joback Method
tc	709.94	K	Joback Method
tf	339.51	K	Joback Method
vc	0.373	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.14	J/molxK	508.68	Joback Method
cpg	203.30	J/molxK	542.22	Joback Method
cpg	210.13	J/molxK	575.77	Joback Method
cpg	216.65	J/molxK	609.31	Joback Method
cpg	222.83	J/molxK	642.86	Joback Method
cpg	228.69	J/molxK	676.40	Joback Method
cpg	234.21	J/molxK	709.94	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=C13558708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13558708&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/55-897-6/Methyl-N-chloroacetylcarbamate.pdf>

Generated by Cheméo on 2024-04-27 03:29:52.327650476 +0000 UTC m=+16477841.248227791.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.