

# Carbamic acid, 3-chlorophenyl-, methyl ester

<b>Inchi:</b>	InChI=1S/C8H8ClNO2/c1-12-8(11)10-7-4-2-3-6(9)5-7/h2-5H,1H3,(H,10,11)
<b>InchiKey:</b>	SEPMCAVKHUPSMA-UHFFFAOYSA-N
<b>Formula:</b>	C8H8ClNO2
<b>SMILES:</b>	COC(=O)Nc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	185.61

## Physical Properties

Property code	Value	Unit	Source
gf	-37.20	kJ/mol	Joback Method
hf	-190.46	kJ/mol	Joback Method
hfus	22.21	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.518		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinsol	1510.00		NIST Webbook
tb	577.99	K	Joback Method
tc	803.50	K	Joback Method
tf	373.60	K	Joback Method
vc	0.483	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.88	J/mol×K	577.99	Joback Method
cpg	290.58	J/mol×K	615.58	Joback Method
cpg	300.59	J/mol×K	653.16	Joback Method
cpg	309.93	J/mol×K	690.75	Joback Method
cpg	318.62	J/mol×K	728.33	Joback Method
cpg	326.67	J/mol×K	765.92	Joback Method
cpg	334.09	J/mol×K	803.50	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=U314750&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U314750&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>rinpol:</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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