

# Methyl 3-chloro-4-methylcarbanilate

<b>Inchi:</b>	InChI=1S/C9H10ClNO2/c1-6-3-4-7(5-8(6)10)11-9(12)13-2/h3-5H,1-2H3,(H,11,12)
<b>InchiKey:</b>	QURFKMPDWGGSOK-UHFFFAOYSA-N
<b>Formula:</b>	C9H10ClNO2
<b>SMILES:</b>	<chem>COC(=O)Nc1ccc(C)c(Cl)c1</chem>
<b>Mol. weight [g/mol]:</b>	199.63
<b>CAS:</b>	22133-20-6

## Physical Properties

Property code	Value	Unit	Source
gf	-38.41	kJ/mol	Joback Method
hf	-222.57	kJ/mol	Joback Method
hfus	24.41	kJ/mol	Joback Method
hvap	59.20	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.827		Crippen Method
mcvol	143.570	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	605.85	K	Joback Method
tc	828.18	K	Joback Method
tf	397.39	K	Joback Method
vc	0.539	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.53	J/molxK	605.85	Joback Method
cpg	335.92	J/molxK	642.91	Joback Method
cpg	346.62	J/molxK	679.96	Joback Method
cpg	356.64	J/molxK	717.02	Joback Method
cpg	365.99	J/molxK	754.07	Joback Method
cpg	374.68	J/molxK	791.13	Joback Method
cpg	382.72	J/molxK	828.18	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=C22133206&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22133206&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>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>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>mccvol:</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

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