

# 1-(2-Chloro-4-methoxyphenyl)-2-methyl-1-propanone

<b>Inchi:</b>	InChI=1S/C11H13ClO2/c1-7(2)11(13)9-5-4-8(14-3)6-10(9)12/h4-7H,1-3H3
<b>InchiKey:</b>	WQBXAJKTQQJVTP-UHFFFAOYSA-N
<b>Formula:</b>	C11H13ClO2
<b>SMILES:</b>	COc1ccc(C(=O)C(C)C)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	212.67
<b>CAS:</b>	116400-86-3

## Physical Properties

Property code	Value	Unit	Source
gf	-113.40	kJ/mol	Joback Method
hf	-322.60	kJ/mol	Joback Method
hfus	20.97	kJ/mol	Joback Method
hvap	56.83	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.187		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	601.00	K	Joback Method
tc	820.90	K	Joback Method
tf	352.27	K	Joback Method
vc	0.611	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.53	J/molxK	601.00	Joback Method
cpg	385.94	J/molxK	637.65	Joback Method
cpg	398.56	J/molxK	674.30	Joback Method
cpg	410.42	J/molxK	710.95	Joback Method
cpg	421.53	J/molxK	747.60	Joback Method
cpg	431.90	J/molxK	784.25	Joback Method
cpg	441.54	J/molxK	820.90	Joback Method
dvisc	0.0015527	Paxs	352.27	Joback Method
dvisc	0.0008920	Paxs	393.72	Joback Method

dvisc	0.0005695	Paxs	435.18	Joback Method
dvisc	0.0003931	Paxs	476.63	Joback Method
dvisc	0.0002880	Paxs	518.09	Joback Method
dvisc	0.0002209	Paxs	559.55	Joback Method
dvisc	0.0001757	Paxs	601.00	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=C116400863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116400863&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>dvisc:</b>	Dynamic viscosity
<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>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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