

# 1-Propanone, 2-chloro-1-(2,4-dimethylphenyl)-2-methyl-

<b>Other names:</b>	2-Chloro-1-(2,4-dimethylphenyl)-2-methyl-1-propanone
<b>Inchi:</b>	InChI=1S/C12H15ClO/c1-8-5-6-10(9(2)7-8)11(14)12(3,4)13/h5-7H,1-4H3
<b>InchiKey:</b>	FRXUQBIZUYXNKL-UHFFFAOYSA-N
<b>Formula:</b>	C12H15ClO
<b>SMILES:</b>	<chem>Cc1ccc(C(=O)C(C)(C)Cl)c(C)c1</chem>
<b>Mol. weight [g/mol]:</b>	210.70
<b>CAS:</b>	54965-53-6

## Physical Properties

Property code	Value	Unit	Source
gf	5.30	kJ/mol	Joback Method
hf	-214.49	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.504		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	598.67	K	Joback Method
tc	826.03	K	Joback Method
tf	358.73	K	Joback Method
vc	0.643	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.09	J/mol×K	598.67	Joback Method
cpg	413.93	J/mol×K	636.56	Joback Method
cpg	427.74	J/mol×K	674.46	Joback Method
cpg	440.58	J/mol×K	712.35	Joback Method
cpg	452.51	J/mol×K	750.24	Joback Method
cpg	463.58	J/mol×K	788.14	Joback Method
cpg	473.87	J/mol×K	826.03	Joback Method
dvisc	0.0018407	Paxs	358.73	Joback Method

dvisc	0.0010437	Paxs	398.72	Joback Method
dvisc	0.0006563	Paxs	438.71	Joback Method
dvisc	0.0004459	Paxs	478.70	Joback Method
dvisc	0.0003216	Paxs	518.69	Joback Method
dvisc	0.0002431	Paxs	558.68	Joback Method
dvisc	0.0001907	Paxs	598.67	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=C54965536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54965536&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>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

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