

# 1-Propanone, 1-(4-chlorophenyl)-

<b>Other names:</b>	Propiophenone, 4'-chloro- p-Chloropropiophenone Ethyl p-chlorophenyl ketone 4-Chloropropiophenone 4'-Chloropropiophenone Propiophenone, p-chloro- USAF EK-5296 1-(4-Chlorophenyl)-1-propanone NSC 5600
<b>Inchi:</b>	InChI=1S/C9H9ClO/c1-2-9(11)7-3-5-8(10)6-4-7/h3-6H,2H2,1H3
<b>InchiKey:</b>	ADCYRBXQAJXJTD-UHFFFAOYSA-N
<b>Formula:</b>	C9H9ClO
<b>SMILES:</b>	CCC(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	168.62
<b>CAS:</b>	6285-05-8

## Physical Properties

Property code	Value	Unit	Source
gf	-13.17	kJ/mol	Joback Method
hf	-132.35	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.933		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	528.28	K	Joback Method
tc	753.10	K	Joback Method
tf	309.98	K	Joback Method
vc	0.486	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	258.49	J/molxK	528.28	Joback Method
cpg	270.24	J/molxK	565.75	Joback Method
cpg	281.24	J/molxK	603.22	Joback Method
cpg	291.51	J/molxK	640.69	Joback Method
cpg	301.10	J/molxK	678.16	Joback Method
cpg	310.02	J/molxK	715.63	Joback Method
cpg	318.31	J/molxK	753.10	Joback Method
dvisc	0.0022080	Paxs	309.98	Joback Method
dvisc	0.0013025	Paxs	346.36	Joback Method
dvisc	0.0008494	Paxs	382.75	Joback Method
dvisc	0.0005966	Paxs	419.13	Joback Method
dvisc	0.0004434	Paxs	455.51	Joback Method
dvisc	0.0003443	Paxs	491.90	Joback Method
dvisc	0.0002769	Paxs	528.28	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	0.10	NIST Webbook
tbrp	408.70	K	4.10	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6285058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6285058&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>
<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>

## 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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