

# 2',4'-dichloropropiophenone

<b>Inchi:</b>	InChI=1S/C9H8Cl2O/c1-2-9(12)7-4-3-6(10)5-8(7)11/h3-5H,2H2,1H3
<b>InchiKey:</b>	FBMTWRZQBRHOPF-UHFFFAOYSA-N
<b>Formula:</b>	C9H8Cl2O
<b>SMILES:</b>	CCC(=O)c1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	203.06
<b>CAS:</b>	37885-41-9

## Physical Properties

Property code	Value	Unit	Source
gf	-34.73	kJ/mol	Joback Method
hf	-159.56	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	54.74	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.586		Crippen Method
mcvol	139.960	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	570.69	K	Joback Method
tc	800.99	K	Joback Method
tf	352.42	K	Joback Method
vc	0.535	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.08	J/molxK	570.69	Joback Method
cpg	327.40	J/molxK	762.61	Joback Method
cpg	319.42	J/molxK	724.23	Joback Method
cpg	310.84	J/molxK	685.84	Joback Method
cpg	301.60	J/molxK	647.46	Joback Method
cpg	291.69	J/molxK	609.07	Joback Method
cpg	334.77	J/molxK	800.99	Joback Method
dvisc	0.0002706	Paxs	570.69	Joback Method
dvisc	0.0003306	Paxs	534.31	Joback Method

dvisc	0.0004158	Paxs	497.93	Joback Method
dvisc	0.0005423	Paxs	461.55	Joback Method
dvisc	0.0007401	Paxs	425.18	Joback Method
dvisc	0.0010705	Paxs	388.80	Joback Method
dvisc	0.0016712	Paxs	352.42	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=C37885419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37885419&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>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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