

# Pivalyl chloride

<b>Other names:</b>	Propanoyl chloride, 2,2-dimethyl- Neopentanoyl chloride Pivalic acid chloride Pivalolyl chloride Pivaloyl chloride Trimethylacetyl chloride 2,2-Dimethylpropanoyl chloride 2,2-Dimethylpropionyl chloride Acetyl chloride, trimethyl- UN 2438 2,2,2-Trimethylacetyl chloride
<b>Inchi:</b>	InChI=1S/C5H9ClO/c1-5(2,3)4(6)7/h1-3H3
<b>InchiKey:</b>	JVSFQJZRHXAUQT-UHFFFAOYSA-N
<b>Formula:</b>	C5H9ClO
<b>SMILES:</b>	CC(C)(C)C(=O)Cl
<b>Mol. weight [g/mol]:</b>	120.58
<b>CAS:</b>	3282-30-2

## Physical Properties

Property code	Value	Unit	Source
gf	-146.79	kJ/mol	Joback Method
hf	-283.60	kJ/mol	Joback Method
hfus	7.09	kJ/mol	Joback Method
hvap	36.56	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.798		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	401.87	K	Joback Method
tc	601.08	K	Joback Method
tf	228.38	K	Joback Method
vc	0.359	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.29	J/molxK	401.87	Joback Method
cpg	211.47	J/molxK	567.88	Joback Method
cpg	203.89	J/molxK	534.68	Joback Method
cpg	195.82	J/molxK	501.47	Joback Method
cpg	187.21	J/molxK	468.27	Joback Method
cpg	178.04	J/molxK	435.07	Joback Method
cpg	218.56	J/molxK	601.08	Joback Method
dvisc	0.0003928	Paxs	401.87	Joback Method
dvisc	0.0005185	Paxs	372.96	Joback Method
dvisc	0.0007172	Paxs	344.04	Joback Method
dvisc	0.0010528	Paxs	315.12	Joback Method
dvisc	0.0016700	Paxs	286.21	Joback Method
dvisc	0.0029388	Paxs	257.30	Joback Method
dvisc	0.0059669	Paxs	228.38	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=C3282302&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3282302&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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