

# 3,3-dimethylbutyryl chloride

<b>Inchi:</b>	InChI=1S/C6H11ClO/c1-6(2,3)4-5(7)8/h4H2,1-3H3
<b>InchiKey:</b>	BUTKIHRNYUEGKB-UHFFFAOYSA-N
<b>Formula:</b>	C6H11ClO
<b>SMILES:</b>	CC(C)(C)CC(=O)Cl
<b>Mol. weight [g/mol]:</b>	134.60
<b>CAS:</b>	7065-46-5

## Physical Properties

Property code	Value	Unit	Source
gf	-138.37	kJ/mol	Joback Method
hf	-304.24	kJ/mol	Joback Method
hfus	9.68	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.188		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	401.20	K	NIST Webbook
tc	622.09	K	Joback Method
tf	239.65	K	Joback Method
vc	0.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.61	J/molxK	424.75	Joback Method
cpg	254.69	J/molxK	589.20	Joback Method
cpg	246.04	J/molxK	556.31	Joback Method
cpg	236.83	J/molxK	523.42	Joback Method
cpg	227.04	J/molxK	490.53	Joback Method
cpg	216.65	J/molxK	457.64	Joback Method
cpg	262.82	J/molxK	622.09	Joback Method
dvisc	0.0003699	Paxs	424.75	Joback Method
dvisc	0.0004907	Paxs	393.90	Joback Method

dvisc	0.0006831	Paxs	363.05	Joback Method
dvisc	0.0010112	Paxs	332.20	Joback Method
dvisc	0.0016221	Paxs	301.35	Joback Method
dvisc	0.0028981	Paxs	270.50	Joback Method
dvisc	0.0060123	Paxs	239.65	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7065465&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7065465&amp;Units=SI</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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