

# Chloromethyl tert-butyl ether

<b>Inchi:</b>	InChI=1S/C5H11ClO/c1-5(2,3)7-4-6/h4H2,1-3H3
<b>InchiKey:</b>	CIACLSGBPZWWNK-UHFFFAOYSA-N
<b>Formula:</b>	C5H11ClO
<b>SMILES:</b>	CC(C)(C)OCCI
<b>Mol. weight [g/mol]:</b>	122.59

## Physical Properties

Property code	Value	Unit	Source
gf	-122.87	kJ/mol	Joback Method
hf	-303.24	kJ/mol	Joback Method
hfus	6.68	kJ/mol	Joback Method
hvap	32.22	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.998		Crippen Method
mvol	99.420	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	772.00		NIST Webbook
rinpol	772.00		NIST Webbook
tb	370.42	K	Joback Method
tc	555.51	K	Joback Method
tf	200.68	K	Joback Method
vc	0.371	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.93	J/molxK	370.42	Joback Method
cpg	184.03	J/molxK	401.27	Joback Method
cpg	193.67	J/molxK	432.12	Joback Method
cpg	202.87	J/molxK	462.97	Joback Method
cpg	211.63	J/molxK	493.82	Joback Method
cpg	219.98	J/molxK	524.67	Joback Method
cpg	227.93	J/molxK	555.51	Joback Method
dvisc	0.0061676	Paxs	200.68	Joback Method

dvisc	0.0027445	Paxs	228.97	Joback Method
dvisc	0.0014593	Paxs	257.26	Joback Method
dvisc	0.0008794	Paxs	285.55	Joback Method
dvisc	0.0005806	Paxs	313.84	Joback Method
dvisc	0.0004106	Paxs	342.13	Joback Method
dvisc	0.0003061	Paxs	370.42	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=R629142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R629142&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>rinpol:</b>	Non-polar retention indices
<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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