

# Butanoic acid, 2-chloro, 1,2-dimethylpropyl ester

Inchi:	InChI=1S/C9H17ClO2/c1-5-8(10)9(11)12-7(4)6(2)3/h6-8H,5H2,1-4H3
InchiKey:	VIMOWINBOFRBHE-UHFFFAOYSA-N
Formula:	C9H17ClO2
SMILES:	CCC(Cl)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	192.68

## Physical Properties

Property code	Value	Unit	Source
gf	-228.27	kJ/mol	Joback Method
hf	-505.47	kJ/mol	Joback Method
hfus	15.48	kJ/mol	Joback Method
hvap	48.00	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.591		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
ripol	1133.00		NIST Webbook
ripol	1129.00		NIST Webbook
ripol	1143.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1124.00		NIST Webbook
ripol	1124.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	517.72	K	Joback Method
tc	708.11	K	Joback Method
tf	248.27	K	Joback Method
vc	0.595	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.90	J/molxK	517.72	Joback Method
cpg	415.98	J/molxK	676.38	Joback Method
cpg	404.54	J/molxK	644.64	Joback Method
cpg	392.53	J/molxK	612.91	Joback Method
cpg	379.92	J/molxK	581.18	Joback Method
cpg	366.71	J/molxK	549.45	Joback Method
cpg	426.84	J/molxK	708.11	Joback Method
dvisc	0.0002020	Paxs	517.72	Joback Method
dvisc	0.0002817	Paxs	472.81	Joback Method
dvisc	0.0004210	Paxs	427.90	Joback Method
dvisc	0.0006916	Paxs	383.00	Joback Method
dvisc	0.0012960	Paxs	338.09	Joback Method
dvisc	0.0029439	Paxs	293.18	Joback Method
dvisc	0.0089985	Paxs	248.27	Joback Method

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R28568&Units=SI>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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