

# Butanoic acid, 4-chloro, butyl ester

<b>Other names:</b>	Butyl 4-chlorobutanoate n-Butyl-4-chlorobutyrate
<b>Inchi:</b>	InChI=1S/C8H15ClO2/c1-2-3-7-11-8(10)5-4-6-9/h2-7H2,1H3
<b>InchiKey:</b>	GKEGQZISIPAXAX-UHFFFAOYSA-N
<b>Formula:</b>	C8H15ClO2
<b>SMILES:</b>	CCCCOC(=O)CCCCI
<b>Mol. weight [g/mol]:</b>	178.66
<b>CAS:</b>	3153-33-1

## Physical Properties

Property code	Value	Unit	Source
chl	-4697.40 ± 8.40	kJ/mol	NIST Webbook
chl	-4688.60	kJ/mol	NIST Webbook
gf	-229.37	kJ/mol	Joback Method
hf	-563.60 ± 9.60	kJ/mol	NIST Webbook
hfl	-618.00 ± 8.40	kJ/mol	NIST Webbook
hfus	23.46	kJ/mol	Joback Method
hvap	54.40 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.349		Crippen Method
mvol	143.260	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1202.00		NIST Webbook
tb	496.16	K	Joback Method
tc	677.00	K	Joback Method
tf	282.00	K	Joback Method
vc	0.556	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	307.66	J/molxK	496.16	Joback Method
cpg	362.34	J/molxK	646.86	Joback Method
cpg	352.32	J/molxK	616.72	Joback Method
cpg	341.84	J/molxK	586.58	Joback Method
cpg	330.91	J/molxK	556.44	Joback Method
cpg	319.52	J/molxK	526.30	Joback Method
cpg	371.92	J/molxK	677.00	Joback Method
dvisc	0.0002618	Paxs	496.16	Joback Method
dvisc	0.0003363	Paxs	460.47	Joback Method
dvisc	0.0004506	Paxs	424.77	Joback Method
dvisc	0.0006370	Paxs	389.08	Joback Method
dvisc	0.0009658	Paxs	353.39	Joback Method
dvisc	0.0016080	Paxs	317.69	Joback Method
dvisc	0.0030458	Paxs	282.00	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=C3153331&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3153331&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>chl:</b>	Standard liquid enthalpy of combustion
<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>hfl:</b>	Liquid phase 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>rinpola:</b>	Non-polar retention indices

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

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