

# Butanoic acid, 2,3-dichloro-, methyl ester

<b>Other names:</b>	Butyric acid, 2,3-dichloro-, methyl ester Methyl threo-2,3-dichlorobutanoate
<b>Inchi:</b>	InChI=1S/C5H8Cl2O2/c1-3(6)4(7)5(8)9-2/h3-4H,1-2H3
<b>InchiKey:</b>	KJZMAXQPXRBYDC-UHFFFAOYSA-N
<b>Formula:</b>	C5H8Cl2O2
<b>SMILES:</b>	COC(=O)C(Cl)C(C)Cl
<b>Mol. weight [g/mol]:</b>	171.02
<b>CAS:</b>	54460-97-8

## Physical Properties

Property code	Value	Unit	Source
gf	-271.44	kJ/mol	Joback Method
hf	-433.37	kJ/mol	Joback Method
hfus	12.84	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.394		Crippen Method
mvol	113.230	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	464.07	K	Joback Method
tc	665.53	K	Joback Method
tf	248.11	K	Joback Method
vc	0.425	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.76	J/mol×K	464.07	Joback Method
cpg	248.84	J/mol×K	631.95	Joback Method
cpg	241.76	J/mol×K	598.37	Joback Method
cpg	234.31	J/mol×K	564.80	Joback Method
cpg	226.49	J/mol×K	531.22	Joback Method
cpg	218.31	J/mol×K	497.65	Joback Method
cpg	255.55	J/mol×K	665.53	Joback Method

dvisc	0.0003006	Paxs	464.07	Joback Method
dvisc	0.0003993	Paxs	428.08	Joback Method
dvisc	0.0005589	Paxs	392.08	Joback Method
dvisc	0.0008373	Paxs	356.09	Joback Method
dvisc	0.0013736	Paxs	320.10	Joback Method
dvisc	0.0025548	Paxs	284.10	Joback Method
dvisc	0.0056889	Paxs	248.11	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=C54460978&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54460978&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>mvol:</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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