

# Methyl 2-bromo-3,3-dichloro-propanoate

<b>Inchi:</b>	InChI=1S/C4H5BrCl2O2/c1-9-4(8)2(5)3(6)7/h2-3H,1H3
<b>InchiKey:</b>	ZRLWLEOCQKMHV-UHFFFAOYSA-N
<b>Formula:</b>	C4H5BrCl2O2
<b>SMILES:</b>	COC(=O)C(Br)C(Cl)Cl
<b>Mol. weight [g/mol]:</b>	235.89

## Physical Properties

Property code	Value	Unit	Source
gf	-265.54	kJ/mol	Joback Method
hf	-386.40	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.727		Crippen Method
mcvol	116.640	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	507.35	K	Joback Method
tc	728.17	K	Joback Method
tf	296.64	K	Joback Method
vc	0.431	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.51	J/molxK	507.35	Joback Method
cpg	229.49	J/molxK	691.37	Joback Method
cpg	224.25	J/molxK	654.57	Joback Method
cpg	218.63	J/molxK	617.76	Joback Method
cpg	212.64	J/molxK	580.96	Joback Method
cpg	206.27	J/molxK	544.15	Joback Method
cpg	234.37	J/molxK	728.17	Joback Method
dvisc	0.0003289	Paxs	507.35	Joback Method
dvisc	0.0004256	Paxs	472.23	Joback Method
dvisc	0.0005740	Paxs	437.11	Joback Method

dvisc	0.0008158	Paxs	402.00	Joback Method
dvisc	0.0012400	Paxs	366.88	Joback Method
dvisc	0.0020594	Paxs	331.76	Joback Method
dvisc	0.0038571	Paxs	296.64	Joback Method

## Sources

<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=U143992&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U143992&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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