

# Propanoic acid, 3-bromo-2-chloro, butyl ester

<b>Inchi:</b>	InChI=1S/C7H12BrClO2/c1-2-3-4-11-7(10)6(9)5-8/h6H,2-5H2,1H3
<b>InchiKey:</b>	JWTFITSDEITTDV-UHFFFAOYSA-N
<b>Formula:</b>	C7H12BrClO2
<b>SMILES:</b>	CCCCOC(=O)C(Cl)CBr
<b>Mol. weight [g/mol]:</b>	243.53

## Physical Properties

Property code	Value	Unit	Source
gf	-225.91	kJ/mol	Joback Method
hf	-427.30	kJ/mol	Joback Method
hfus	22.63	kJ/mol	Joback Method
hvap	50.76	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.332		Crippen Method
mcvol	146.670	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
tb	539.00	K	Joback Method
tc	740.26	K	Joback Method
tf	315.53	K	Joback Method
vc	0.556	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.89	J/molxK	539.00	Joback Method
cpg	349.95	J/molxK	706.72	Joback Method
cpg	341.35	J/molxK	673.17	Joback Method
cpg	332.25	J/molxK	639.63	Joback Method
cpg	322.65	J/molxK	606.09	Joback Method
cpg	312.53	J/molxK	572.54	Joback Method
cpg	358.07	J/molxK	740.26	Joback Method
dvisc	0.0002681	Paxs	539.00	Joback Method

dvisc	0.0003450	Paxs	501.75	Joback Method
dvisc	0.0004623	Paxs	464.51	Joback Method
dvisc	0.0006519	Paxs	427.26	Joback Method
dvisc	0.0009817	Paxs	390.02	Joback Method
dvisc	0.0016119	Paxs	352.77	Joback Method
dvisc	0.0029753	Paxs	315.53	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=R30282&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R30282&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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