

# Butyric acid, 2-bromo-, 1-methylethyl ester

<b>Other names:</b>	Isopropyl 2-bromobutanoate
<b>Inchi:</b>	InChI=1S/C7H13BrO2/c1-4-6(8)7(9)10-5(2)3/h5-6H,4H2,1-3H3
<b>InchiKey:</b>	XSRQGXXVWFDYHQ-TUHFFFAOYSA-N
<b>Formula:</b>	C7H13BrO2
<b>SMILES:</b>	CCC(Br)C(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	209.08

## Physical Properties

Property code	Value	Unit	Source
gf	-216.42	kJ/mol	Joback Method
hf	-416.84	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.111		Crippen Method
mvol	134.430	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1033.00		NIST Webbook
tb	501.13	K	Joback Method
tc	701.72	K	Joback Method
tf	270.61	K	Joback Method
vc	0.501	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.34	J/molxK	501.13	Joback Method
cpg	288.87	J/molxK	534.56	Joback Method
cpg	299.87	J/molxK	567.99	Joback Method
cpg	310.34	J/molxK	601.42	Joback Method
cpg	320.30	J/molxK	634.85	Joback Method
cpg	329.75	J/molxK	668.28	Joback Method
cpg	338.71	J/molxK	701.72	Joback Method
dvisc	0.0047978	Paxs	270.61	Joback Method

dvisc	0.0021989	Paxs	309.03	Joback Method
dvisc	0.0011975	Paxs	347.45	Joback Method
dvisc	0.0007361	Paxs	385.87	Joback Method
dvisc	0.0004941	Paxs	424.29	Joback Method
dvisc	0.0003544	Paxs	462.71	Joback Method
dvisc	0.0002675	Paxs	501.13	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=U131992&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U131992&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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