

# Butyric acid, 2-bromo-, propyl ester

<b>Other names:</b>	Propyl 2-bromobutanoate
<b>Inchi:</b>	InChI=1S/C7H13BrO2/c1-3-5-10-7(9)6(8)4-2/h6H,3-5H2,1-2H3
<b>InchiKey:</b>	BJPYPGKBFMZGDQ-UHFFFAOYSA-N
<b>Formula:</b>	C7H13BrO2
<b>SMILES:</b>	CCCOC(=O)C(Br)CC
<b>Mol. weight [g/mol]:</b>	209.08
<b>CAS:</b>	5459-97-2

## Physical Properties

Property code	Value	Unit	Source
gf	-213.98	kJ/mol	Joback Method
hf	-411.56	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.113		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1089.00		NIST Webbook
tb	501.57	K	Joback Method
tc	697.81	K	Joback Method
tf	285.61	K	Joback Method
vc	0.507	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.07	J/molxK	501.57	Joback Method
cpg	328.18	J/molxK	665.11	Joback Method
cpg	318.93	J/molxK	632.40	Joback Method
cpg	309.20	J/molxK	599.69	Joback Method
cpg	298.99	J/molxK	566.98	Joback Method
cpg	288.28	J/molxK	534.28	Joback Method
cpg	336.97	J/molxK	697.81	Joback Method

dvisc	0.0002828	Paxs	501.57	Joback Method
dvisc	0.0003653	Paxs	465.58	Joback Method
dvisc	0.0004925	Paxs	429.58	Joback Method
dvisc	0.0007013	Paxs	393.59	Joback Method
dvisc	0.0010723	Paxs	357.60	Joback Method
dvisc	0.0018031	Paxs	321.60	Joback Method
dvisc	0.0034561	Paxs	285.61	Joback Method

## Sources

<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>
<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=C5459972&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5459972&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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