

# 3-bromobutyric acid

<b>Other names:</b>	Butanoic acid, 3-bromo-
<b>Inchi:</b>	InChI=1S/C4H7BrO2/c1-3(5)2-4(6)7/h3H,2H2,1H3,(H,6,7)
<b>InchiKey:</b>	HAIUIAZIUDPZIE-UHFFFAOYSA-N
<b>Formula:</b>	C4H7BrO2
<b>SMILES:</b>	CC(Br)CC(=O)O
<b>Mol. weight [g/mol]:</b>	167.00
<b>CAS:</b>	2623-86-1

## Physical Properties

Property code	Value	Unit	Source
gf	-271.06	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.244		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	502.69	K	Joback Method
tc	696.12	K	Joback Method
tf	290.39	K	Joback Method
vc	0.341	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.75	J/mol×K	502.69	Joback Method
cpg	203.74	J/mol×K	663.89	Joback Method
cpg	198.57	J/mol×K	631.65	Joback Method
cpg	193.11	J/mol×K	599.41	Joback Method
cpg	187.32	J/mol×K	567.17	Joback Method
cpg	181.21	J/mol×K	534.93	Joback Method
cpg	208.61	J/mol×K	696.12	Joback Method
dvisc	0.0002386	Paxs	502.69	Joback Method

dvisc	0.0003734	Paxs	467.31	Joback Method
dvisc	0.0006292	Paxs	431.92	Joback Method
dvisc	0.0011634	Paxs	396.54	Joback Method
dvisc	0.0024265	Paxs	361.16	Joback Method
dvisc	0.0059375	Paxs	325.77	Joback Method
dvisc	0.0180688	Paxs	290.39	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.00	K	2.10	NIST Webbook

## 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=C2623861&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623861&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>

## 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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