

# Butanenitrile, 4-bromo-

<b>Other names:</b>	Butyronitrile, 4-bromo- «gamma»-Bromobutyronitrile 3-Bromopropyl cyanide 3-Cyanopropyl bromide 4-Bromobutyronitrile USAF DO-6 4-Bromobutanenitrile gamma-Bromobutyronitrile 1-Bromo-3-cyanopropane NSC 3972
<b>Inchi:</b>	InChI=1S/C4H6BrN/c5-3-1-2-4-6/h1-3H2
<b>InchiKey:</b>	CQPGDDAKTTWVDD-UHFFFAOYSA-N
<b>Formula:</b>	C4H6BrN
<b>SMILES:</b>	N#CCCCBr
<b>Mol. weight [g/mol]:</b>	148.00
<b>CAS:</b>	5332-06-9

## Physical Properties

Property code	Value	Unit	Source
gf	130.30	kJ/mol	Joback Method
hf	65.32	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	41.41	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.685		Crippen Method
mcvol	86.100	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
tb	479.20	K	NIST Webbook
tc	670.20	K	Joback Method
tf	259.63	K	Joback Method
vc	0.347	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.11	J/mol×K	459.16	Joback Method
cpg	151.35	J/mol×K	494.33	Joback Method
cpg	157.24	J/mol×K	529.51	Joback Method
cpg	162.80	J/mol×K	564.68	Joback Method
cpg	168.06	J/mol×K	599.85	Joback Method
cpg	173.02	J/mol×K	635.03	Joback Method
cpg	177.70	J/mol×K	670.20	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.20	K	1.60	NIST Webbook

## 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=C5332069&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5332069&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</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>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>hvp:</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

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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