

# Acetonitrile, bromochloro-

<b>Other names:</b>	Bromochloroacetonitrile Bromochloromethyl cyanide
<b>Inchi:</b>	InChI=1S/C2HBrCIN/c3-2(4)1-5/h2H
<b>InchiKey:</b>	BMWPPNAUMLRKML-UHFFFAOYSA-N
<b>Formula:</b>	C2HBrCIN
<b>SMILES:</b>	N#CC(Cl)Br
<b>Mol. weight [g/mol]:</b>	154.39
<b>CAS:</b>	83463-62-1

## Physical Properties

Property code	Value	Unit	Source
gf	99.09	kJ/mol	Joback Method
hf	85.58	kJ/mol	Joback Method
hfus	8.40	kJ/mol	Joback Method
hvap	40.96	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.470		Crippen Method
mvol	70.160	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	758.00		NIST Webbook
rinpol	758.00		NIST Webbook
tb	450.39	K	Joback Method
tc	679.74	K	Joback Method
tf	252.01	K	Joback Method
vc	0.279	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.56	J/mol×K	450.39	Joback Method
cpg	95.31	J/mol×K	488.61	Joback Method
cpg	97.83	J/mol×K	526.84	Joback Method
cpg	100.15	J/mol×K	565.06	Joback Method
cpg	102.27	J/mol×K	603.29	Joback Method

cpg	104.21	J/mol×K	641.51	Joback Method
cpg	106.00	J/mol×K	679.74	Joback Method

## 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=C83463621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C83463621&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>
<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>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>rinpola:</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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