

# Acetonitrile, dibromo-

<b>Other names:</b>	Dibromoacetonitrile
<b>Inchi:</b>	InChI=1S/C2HBr2N/c3-2(4)1-5/h2H
<b>InchiKey:</b>	NDSBDLSWTGLNQA-UHFFFAOYSA-N
<b>Formula:</b>	C2HBr2N
<b>SMILES:</b>	N#CC(Br)Br
<b>Mol. weight [g/mol]:</b>	198.84
<b>CAS:</b>	3252-43-5

## Physical Properties

Property code	Value	Unit	Source
gf	125.34	kJ/mol	Joback Method
hf	127.65	kJ/mol	Joback Method
hfus	9.49	kJ/mol	Joback Method
hvap	43.01	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.626		Crippen Method
mcvol	75.420	ml/mol	McGowan Method
pc	6018.58	kPa	Joback Method
rinpol	861.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	853.30		NIST Webbook
rinpol	853.30		NIST Webbook
tb	479.12	K	Joback Method
tc	720.72	K	Joback Method
tf	281.89	K	Joback Method
vc	0.291	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.04	J/molxK	479.12	Joback Method
cpg	98.72	J/molxK	519.39	Joback Method

cpg	101.13	J/mol×K	559.65	Joback Method
cpg	103.29	J/mol×K	599.92	Joback Method
cpg	105.23	J/mol×K	640.18	Joback Method
cpg	106.99	J/mol×K	680.45	Joback Method
cpg	108.59	J/mol×K	720.72	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	3.20	NIST Webbook

## Sources

<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=C3252435&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3252435&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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