

# Bromonitromethane

<b>Other names:</b>	Methane, bromonitro-
<b>Inchi:</b>	InChI=1S/CH2BrNO2/c2-1-3(4)5/h1H2
<b>InchiKey:</b>	DNPRVXJGNANVCZ-UHFFFAOYSA-N
<b>Formula:</b>	CH2BrNO2
<b>SMILES:</b>	O=[N+](O-)CBr
<b>Mol. weight [g/mol]:</b>	139.94
<b>CAS:</b>	563-70-2

## Physical Properties

Property code	Value	Unit	Source
gf	7.41	kJ/mol	Joback Method
hf	-48.40	kJ/mol	Joback Method
hfus	14.99	kJ/mol	Joback Method
hvap	40.85	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	0.615		Crippen Method
mcvol	59.870	ml/mol	McGowan Method
pc	6577.70	kPa	Joback Method
tb	440.28	K	Joback Method
tc	675.81	K	Joback Method
tf	304.44	K	Joback Method
vc	0.235	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.42	J/molxK	440.28	Joback Method
cpg	93.54	J/molxK	479.54	Joback Method
cpg	97.35	J/molxK	518.79	Joback Method
cpg	100.87	J/molxK	558.05	Joback Method
cpg	104.11	J/molxK	597.30	Joback Method
cpg	107.10	J/molxK	636.56	Joback Method
cpg	109.86	J/molxK	675.81	Joback Method

# 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=C563702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C563702&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>

# 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>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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