

# 2-Bromo-2-nitropropane

<b>Other names:</b>	Propane, 2-bromo-2-nitro-
<b>Inchi:</b>	InChI=1S/C3H6BrNO2/c1-3(2,4)5(6)7/h1-2H3
<b>InchiKey:</b>	OADSZWXMXIWZSQ-UHFFFAOYSA-N
<b>Formula:</b>	C3H6BrNO2
<b>SMILES:</b>	CC(C)(Br)[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	167.99
<b>CAS:</b>	5447-97-2

## Physical Properties

Property code	Value	Unit	Source
gf	27.09	kJ/mol	Joback Method
hf	-98.43	kJ/mol	Joback Method
hfus	12.76	kJ/mol	Joback Method
hvap	44.00	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.394		Crippen Method
mcvol	88.050	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	482.81	K	Joback Method
tc	726.86	K	Joback Method
tf	329.40	K	Joback Method
vc	0.337	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.43	J/molxK	482.81	Joback Method
cpg	173.67	J/molxK	523.49	Joback Method
cpg	181.16	J/molxK	564.16	Joback Method
cpg	187.97	J/molxK	604.84	Joback Method
cpg	194.16	J/molxK	645.51	Joback Method
cpg	199.78	J/molxK	686.19	Joback Method
cpg	204.90	J/molxK	726.86	Joback Method

# 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=C5447972&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5447972&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>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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