

# 2-Nitrobenzyl bromide

<b>Other names:</b>	o-Nitrobenzyl bromide Benzene, 1-(bromomethyl)-2-nitro- «alpha»-bromo-2-nitrotoluene
<b>Inchi:</b>	InChI=1S/C7H6BrNO2/c8-5-6-3-1-2-4-7(6)9(10)11/h1-4H,5H2
<b>InchiKey:</b>	HXBMIQJOSHZCFX-UHFFFAOYSA-N
<b>Formula:</b>	C7H6BrNO2
<b>SMILES:</b>	O=[N+](O-)c1cccc1CBr
<b>Mol. weight [g/mol]:</b>	216.03
<b>CAS:</b>	3958-60-9

## Physical Properties

Property code	Value	Unit	Source
gf	160.71	kJ/mol	Joback Method
hf	52.82	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	57.14	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.490		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	609.22	K	Joback Method
tc	873.25	K	Joback Method
tf	411.00	K	Joback Method
vc	0.464	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.36	J/molxK	609.22	Joback Method
cpg	261.26	J/molxK	653.23	Joback Method
cpg	270.29	J/molxK	697.23	Joback Method
cpg	278.52	J/molxK	741.24	Joback Method
cpg	286.01	J/molxK	785.24	Joback Method
cpg	292.84	J/molxK	829.25	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=C3958609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3958609&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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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