

# Benzenemethanol, 4-bromo-

<b>Other names:</b>	Benzyl alcohol, p-bromo- p-Bromobenzyl alcohol 4-Bromobenzyl alcohol
<b>Inchi:</b>	InChI=1S/C7H7BrO/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2
<b>InchiKey:</b>	VEDDBHYQWFOITD-UHFFFAOYSA-N
<b>Formula:</b>	C7H7BrO
<b>SMILES:</b>	OCc1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	187.03
<b>CAS:</b>	873-75-6

## Physical Properties

Property code	Value	Unit	Source
gf	-11.66	kJ/mol	Joback Method
hf	-88.65	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.941		Crippen Method
mcvol	109.100	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	549.56	K	Joback Method
tc	765.72	K	Joback Method
tf	328.21	K	Joback Method
vc	0.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.18	J/mol×K	549.56	Joback Method
cpg	250.21	J/mol×K	729.69	Joback Method
cpg	243.80	J/mol×K	693.66	Joback Method
cpg	236.93	J/mol×K	657.64	Joback Method
cpg	229.56	J/mol×K	621.61	Joback Method
cpg	221.65	J/mol×K	585.59	Joback Method

cpg	256.18	J/mol×K	765.72	Joback Method
dvisc	0.0001406	Paxs	549.56	Joback Method
dvisc	0.0002070	Paxs	512.67	Joback Method
dvisc	0.0003238	Paxs	475.78	Joback Method
dvisc	0.0005458	Paxs	438.88	Joback Method
dvisc	0.0010127	Paxs	401.99	Joback Method
dvisc	0.0021291	Paxs	365.10	Joback Method
dvisc	0.0052897	Paxs	328.21	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C873756&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C873756&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>
<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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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