

# 3-Bromo-4-methoxyphenylacetonitrile

<b>Inchi:</b>	InChI=1S/C9H8BrNO/c1-12-9-3-2-7(4-5-11)6-8(9)10/h2-3,6H,4H2,1H3
<b>InchiKey:</b>	OBJKHHRZMII EOK-UHFFFAOYSA-N
<b>Formula:</b>	C9H8BrNO
<b>SMILES:</b>	COc1ccc(CC#N)cc1Br
<b>Mol. weight [g/mol]:</b>	226.07
<b>CAS:</b>	772-59-8

## Physical Properties

Property code	Value	Unit	Source
gf	160.55	kJ/mol	Joback Method
hf	43.49	kJ/mol	Joback Method
hfus	20.31	kJ/mol	Joback Method
hvap	58.55	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.524		Crippen Method
mcvol	138.660	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	632.62	K	Joback Method
tc	872.07	K	Joback Method
tf	389.67	K	Joback Method
vc	0.537	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.44	J/molxK	632.62	Joback Method
cpg	305.27	J/molxK	672.53	Joback Method
cpg	314.45	J/molxK	712.44	Joback Method
cpg	323.00	J/molxK	752.35	Joback Method
cpg	330.95	J/molxK	792.26	Joback Method
cpg	338.29	J/molxK	832.16	Joback Method
cpg	345.07	J/molxK	872.07	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C772598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C772598&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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