

# Benzamide, m-bromo-

<b>Other names:</b>	Benzamide, 3-bromo- 3-bromobenzamide
<b>Inchi:</b>	InChI=1S/C7H6BrNO/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H2,9,10)
<b>InchiKey:</b>	ODJFDWIECLJWSR-UHFFFAOYSA-N
<b>Formula:</b>	C7H6BrNO
<b>SMILES:</b>	NC(=O)c1cccc(Br)c1
<b>Mol. weight [g/mol]:</b>	200.03
<b>CAS:</b>	22726-00-7

## Physical Properties

Property code	Value	Unit	Source
gf	62.69	kJ/mol	Joback Method
hf	-15.21	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.548		Crippen Method
mvol	114.780	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
tb	583.78	K	Joback Method
tc	837.04	K	Joback Method
tf	400.58	K	Joback Method
vc	0.416	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.12	J/molxK	583.78	Joback Method
cpg	239.29	J/molxK	625.99	Joback Method
cpg	247.70	J/molxK	668.20	Joback Method
cpg	255.39	J/molxK	710.41	Joback Method
cpg	262.43	J/molxK	752.62	Joback Method
cpg	268.85	J/molxK	794.83	Joback Method
cpg	274.71	J/molxK	837.04	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=C22726007&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22726007&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>

# 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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