

# Benzamide, N-(4-bromophenyl)-3-bromo-

<b>Inchi:</b>	InChI=1S/C13H9Br2NO/c14-10-4-6-12(7-5-10)16-13(17)9-2-1-3-11(15)8-9/h1-8H,(H,16,17)
<b>InchiKey:</b>	RNMIDZORNPWDTP-UHFFFAOYSA-N
<b>Formula:</b>	C13H9Br2NO
<b>SMILES:</b>	O=C(Nc1ccc(Br)cc1)c1cccc(Br)c1
<b>Mol. weight [g/mol]:</b>	355.02

## Physical Properties

Property code	Value	Unit	Source
gf	253.25	kJ/mol	Joback Method
hf	132.02	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.464		Crippen Method
mcvol	193.060	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpola	2559.00		NIST Webbook
rinpola	2559.00		NIST Webbook
tb	796.52	K	Joback Method
tc	1067.35	K	Joback Method
tf	536.34	K	Joback Method
vc	0.713	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.54	J/mol×K	796.52	Joback Method
cpg	461.07	J/mol×K	841.66	Joback Method
cpg	470.60	J/mol×K	886.80	Joback Method
cpg	479.26	J/mol×K	931.93	Joback Method
cpg	487.17	J/mol×K	977.07	Joback Method
cpg	494.43	J/mol×K	1022.21	Joback Method
cpg	501.19	J/mol×K	1067.35	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307156&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307156&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>

# 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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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