

# Benzamide, N-decyl-N-methyl-4-bromo-

<b>Inchi:</b>	InChI=1S/C18H28BrNO/c1-3-4-5-6-7-8-9-10-15-20(2)18(21)16-11-13-17(19)14-12-16/h1
<b>InchiKey:</b>	IVSUQHPPAYILPU-UHFFFAOYSA-N
<b>Formula:</b>	C18H28BrNO
<b>SMILES:</b>	CCCCCCCCCN(C)C(=O)c1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	354.32

## Physical Properties

Property code	Value	Unit	Source
gf	199.64	kJ/mol	Joback Method
hf	-208.51	kJ/mol	Joback Method
hfus	45.93	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.662		Crippen Method
mcvol	269.770	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinsol	2490.00		NIST Webbook
tb	775.37	K	Joback Method
tc	977.89	K	Joback Method
tf	473.76	K	Joback Method
vc	1.022	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.11	J/mol×K	775.37	Joback Method
cpg	785.71	J/mol×K	809.12	Joback Method
cpg	801.30	J/mol×K	842.88	Joback Method
cpg	815.96	J/mol×K	876.63	Joback Method
cpg	829.73	J/mol×K	910.38	Joback Method
cpg	842.69	J/mol×K	944.13	Joback Method
cpg	854.90	J/mol×K	977.89	Joback Method

# Sources

<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>
<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=U308454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308454&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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