

# Benzamide, N,N-diheptyl-3-bromo-

<b>Inchi:</b>	InChI=1S/C21H34BrNO/c1-3-5-7-9-11-16-23(17-12-10-8-6-4-2)21(24)19-14-13-15-20(22)
<b>InchiKey:</b>	TXRYYWOQIWGWTC-UHFFFAOYSA-N
<b>Formula:</b>	C21H34BrNO
<b>SMILES:</b>	CCCCCCCN(CCCCCC)C(=O)c1cccc(Br)c1
<b>Mol. weight [g/mol]:</b>	396.40

## Physical Properties

Property code	Value	Unit	Source
gf	224.90	kJ/mol	Joback Method
hf	-270.43	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.832		Crippen Method
mcvol	312.040	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpola	2532.00		NIST Webbook
rinpola	2532.00		NIST Webbook
tb	844.01	K	Joback Method
tc	1045.57	K	Joback Method
tf	507.57	K	Joback Method
vc	1.190	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.83	J/molxK	844.01	Joback Method
cpg	962.19	J/molxK	877.60	Joback Method
cpg	978.53	J/molxK	911.20	Joback Method
cpg	993.91	J/molxK	944.79	Joback Method
cpg	1008.40	J/molxK	978.39	Joback Method
cpg	1022.08	J/molxK	1011.98	Joback Method
cpg	1035.01	J/molxK	1045.57	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=U308625&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308625&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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