

# Pentanamide, N,N-dihexyl-5-bromo-

<b>Inchi:</b>	InChI=1S/C17H34BrNO/c1-3-5-7-11-15-19(16-12-8-6-4-2)17(20)13-9-10-14-18/h3-16H2,
<b>InchiKey:</b>	GWPLZVXNYGPQPK-UHFFFAOYSA-N
<b>Formula:</b>	C17H34BrNO
<b>SMILES:</b>	CCCCCN(CCCCCC)C(=O)CCCCBr
<b>Mol. weight [g/mol]:</b>	348.36

## Physical Properties

Property code	Value	Unit	Source
gf	88.44	kJ/mol	Joback Method
hf	-412.93	kJ/mol	Joback Method
hfus	49.69	kJ/mol	Joback Method
hvap	68.66	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.541		Crippen Method
mvol	279.440	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2264.00		NIST Webbook
tb	720.83	K	Joback Method
tc	898.74	K	Joback Method
tf	423.55	K	Joback Method
vc	1.073	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.79	J/mol×K	720.83	Joback Method
cpg	814.46	J/mol×K	750.48	Joback Method
cpg	831.25	J/mol×K	780.13	Joback Method
cpg	847.22	J/mol×K	809.79	Joback Method
cpg	862.39	J/mol×K	839.44	Joback Method
cpg	876.81	J/mol×K	869.09	Joback Method
cpg	890.52	J/mol×K	898.74	Joback Method

# Sources

<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=U308260&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308260&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>

# 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>rinpola:</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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