

# Bromoacetamide, N,N-diheptyl-

<b>Inchi:</b>	InChI=1S/C16H32BrNO/c1-3-5-7-9-11-13-18(16(19)15-17)14-12-10-8-6-4-2/h3-15H2,1-2
<b>InchiKey:</b>	KYQUVIIYMPDQEZ-UHFFFAOYSA-N
<b>Formula:</b>	C16H32BrNO
<b>SMILES:</b>	CCCCCCCN(CCCCCC)C(=O)CBr
<b>Mol. weight [g/mol]:</b>	334.33

## Physical Properties

Property code	Value	Unit	Source
gf	80.02	kJ/mol	Joback Method
hf	-392.29	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	66.43	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	5.151		Crippen Method
mcvol	265.350	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinqol	2157.00		NIST Webbook
tb	697.95	K	Joback Method
tc	875.62	K	Joback Method
tf	412.28	K	Joback Method
vc	1.018	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.59	J/molxK	697.95	Joback Method
cpg	756.88	J/molxK	727.56	Joback Method
cpg	773.32	J/molxK	757.17	Joback Method
cpg	788.95	J/molxK	786.78	Joback Method
cpg	803.80	J/molxK	816.40	Joback Method
cpg	817.91	J/molxK	846.01	Joback Method
cpg	831.33	J/molxK	875.62	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=U308171&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308171&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>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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