

# Bromacetamide, N-dodecyl-

<b>Inchi:</b>	InChI=1S/C14H28BrNO/c1-2-3-4-5-6-7-8-9-10-11-12-16-14(17)13-15/h2-13H2,1H3,(H,16)
<b>InchiKey:</b>	PYTFETBMLNNDNW-UHFFFAOYSA-N
<b>Formula:</b>	C14H28BrNO
<b>SMILES:</b>	CCCCCCCCCCCCNC(=O)CBr
<b>Mol. weight [g/mol]:</b>	306.28

## Physical Properties

Property code	Value	Unit	Source
gf	41.79	kJ/mol	Joback Method
hf	-365.07	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.418		Crippen Method
mvol	237.170	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	689.92	K	Joback Method
tc	872.27	K	Joback Method
tf	409.93	K	Joback Method
vc	0.922	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.65	J/molxK	689.92	Joback Method
cpg	663.50	J/molxK	720.31	Joback Method
cpg	678.57	J/molxK	750.70	Joback Method
cpg	692.89	J/molxK	781.09	Joback Method
cpg	706.48	J/molxK	811.49	Joback Method
cpg	719.38	J/molxK	841.88	Joback Method
cpg	731.62	J/molxK	872.27	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=U407081&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407081&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>
<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>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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