

# Bromoacetamide, N,N-dioctyl-

<b>Inchi:</b>	InChI=1S/C18H36BrNO/c1-3-5-7-9-11-13-15-20(18(21)17-19)16-14-12-10-8-6-4-2/h3-17
<b>InchiKey:</b>	XEFDAMQSIJLBRD-UHFFFAOYSA-N
<b>Formula:</b>	C18H36BrNO
<b>SMILES:</b>	CCCCCCCCN(CCCCCCCC)C(=O)CBr
<b>Mol. weight [g/mol]:</b>	362.39

## Physical Properties

Property code	Value	Unit	Source
gf	96.86	kJ/mol	Joback Method
hf	-433.57	kJ/mol	Joback Method
hfus	52.28	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.931		Crippen Method
mcvol	293.530	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinsol	2366.00		NIST Webbook
tb	743.71	K	Joback Method
tc	922.40	K	Joback Method
tf	434.82	K	Joback Method
vc	1.129	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.05	J/mol×K	743.71	Joback Method
cpg	873.10	J/mol×K	773.49	Joback Method
cpg	890.25	J/mol×K	803.27	Joback Method
cpg	906.54	J/mol×K	833.05	Joback Method
cpg	922.03	J/mol×K	862.83	Joback Method
cpg	936.75	J/mol×K	892.62	Joback Method
cpg	950.74	J/mol×K	922.40	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=U308173&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308173&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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