

# Chloroacetamide, N,N-diheptyl-

<b>Inchi:</b>	InChI=1S/C16H32ClNO/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>	ZOFPQFIAAZHFAY-UHFFFAOYSA-N
<b>Formula:</b>	C16H32ClNO
<b>SMILES:</b>	CCCCCCCN(CCCCCC)C(=O)CCl
<b>Mol. weight [g/mol]:</b>	289.88

## Physical Properties

Property code	Value	Unit	Source
gf	53.77	kJ/mol	Joback Method
hf	-434.36	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.995		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	669.22	K	Joback Method
tc	840.41	K	Joback Method
tf	382.40	K	Joback Method
vc	1.004	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.98	J/mol×K	669.22	Joback Method
cpg	738.57	J/mol×K	697.75	Joback Method
cpg	755.33	J/mol×K	726.28	Joback Method
cpg	771.30	J/mol×K	754.82	Joback Method
cpg	786.51	J/mol×K	783.35	Joback Method
cpg	800.97	J/mol×K	811.88	Joback Method
cpg	814.74	J/mol×K	840.41	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=U308478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308478&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>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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