

# Valeramide, 5-chloro-N-(5-chlorovaleryl)-N-hexyl-

<b>Inchi:</b>	InChI=1S/C16H29Cl2NO2/c1-2-3-4-9-14-19(15(20)10-5-7-12-17)16(21)11-6-8-13-18/h2-
<b>InchiKey:</b>	AQBXHVHEIJYJDC-UHFFFAOYSA-N
<b>Formula:</b>	C16H29Cl2NO2
<b>SMILES:</b>	CCCCCN(C(=O)CCCCCl)C(=O)CCCCCl
<b>Mol. weight [g/mol]:</b>	338.31

## Physical Properties

Property code	Value	Unit	Source
gf	-87.08	kJ/mol	Joback Method
hf	-562.68	kJ/mol	Joback Method
hfus	51.81	kJ/mol	Joback Method
hvap	75.52	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.740		Crippen Method
mvol	273.900	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2438.00		NIST Webbook
tb	760.52	K	Joback Method
tc	944.78	K	Joback Method
tf	462.25	K	Joback Method
vc	1.060	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.51	J/mol×K	760.52	Joback Method
cpg	792.95	J/mol×K	791.23	Joback Method
cpg	807.54	J/mol×K	821.94	Joback Method
cpg	821.33	J/mol×K	852.65	Joback Method
cpg	834.34	J/mol×K	883.36	Joback Method
cpg	846.62	J/mol×K	914.07	Joback Method
cpg	858.20	J/mol×K	944.78	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=U407544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407544&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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