

# Benzamide, 3-chloro-N-hexyl-

<b>Inchi:</b>	InChI=1S/C13H18ClNO/c1-2-3-4-5-9-15-13(16)11-7-6-8-12(14)10-11/h6-8,10H,2-5,9H2,1
<b>InchiKey:</b>	MIWJVAHFQPNBEW-UHFFFAOYSA-N
<b>Formula:</b>	C13H18ClNO
<b>SMILES:</b>	CCCCCCNC(=O)c1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	239.74

## Physical Properties

Property code	Value	Unit	Source
gf	109.90	kJ/mol	Joback Method
hf	-161.44	kJ/mol	Joback Method
hfus	33.97	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.650		Crippen Method
mvol	194.060	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	669.97	K	Joback Method
tc	879.44	K	Joback Method
tf	407.72	K	Joback Method
vc	0.746	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.84	J/mol×K	669.97	Joback Method
cpg	512.33	J/mol×K	704.88	Joback Method
cpg	525.92	J/mol×K	739.79	Joback Method
cpg	538.64	J/mol×K	774.70	Joback Method
cpg	550.54	J/mol×K	809.62	Joback Method
cpg	561.65	J/mol×K	844.53	Joback Method
cpg	572.02	J/mol×K	879.44	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U407979&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407979&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>hvp:</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>rinp:</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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