

# Benzamide, 4-chloro-N-ethyl-N-hexyl-

<b>Inchi:</b>	InChI=1S/C15H22ClNO/c1-3-5-6-7-12-17(4-2)15(18)13-8-10-14(16)11-9-13/h8-11H,3-7,1
<b>InchiKey:</b>	VQMKLZIXOHZRIZ-UHFFFAOYSA-N
<b>Formula:</b>	C15H22ClNO
<b>SMILES:</b>	CCCCCN(CC)C(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	267.79

## Physical Properties

Property code	Value	Unit	Source
gf	148.13	kJ/mol	Joback Method
hf	-188.66	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.382		Crippen Method
mvol	222.240	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	678.00	K	Joback Method
tc	879.41	K	Joback Method
tf	410.07	K	Joback Method
vc	0.841	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.50	J/mol×K	678.00	Joback Method
cpg	603.63	J/mol×K	711.57	Joback Method
cpg	618.79	J/mol×K	745.14	Joback Method
cpg	633.02	J/mol×K	778.71	Joback Method
cpg	646.37	J/mol×K	812.28	Joback Method
cpg	658.89	J/mol×K	845.85	Joback Method
cpg	670.61	J/mol×K	879.41	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.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=U415327&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415327&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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