

# Heptananilide, 3'-chloro-6-methyl-

<b>Inchi:</b>	InChI=1S/C14H20ClNO/c1-11(2)6-3-4-9-14(17)16-13-8-5-7-12(15)10-13/h5,7-8,10-11H,3
<b>InchiKey:</b>	ABRVPKIHYGSJOU-UHFFFAOYSA-N
<b>Formula:</b>	C14H20ClNO
<b>SMILES:</b>	CC(C)CCCC(=O)Nc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	253.77
<b>CAS:</b>	116435-55-3

## Physical Properties

Property code	Value	Unit	Source
gf	115.88	kJ/mol	Joback Method
hf	-187.36	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.495		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
tb	692.41	K	Joback Method
tc	902.61	K	Joback Method
tf	403.99	K	Joback Method
vc	0.795	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.72	J/mol×K	692.41	Joback Method
cpg	565.95	J/mol×K	727.44	Joback Method
cpg	580.21	J/mol×K	762.48	Joback Method
cpg	593.55	J/mol×K	797.51	Joback Method
cpg	606.01	J/mol×K	832.54	Joback Method
cpg	617.63	J/mol×K	867.57	Joback Method
cpg	628.46	J/mol×K	902.61	Joback Method

# Sources

<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=C116435553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116435553&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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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