

# 4-Chloro-3-nitrobenzanilide

<b>Other names:</b>	Benzamide, 4-chloro-3-nitro-N-phenyl- 4-Chloro-3-nitro-N-phenylbenzamide
<b>Inchi:</b>	InChI=1S/C13H9ClN2O3/c14-11-7-6-9(8-12(11)16(18)19)13(17)15-10-4-2-1-3-5-10/h1-8
<b>InchiKey:</b>	MPSDMWLZVDJFGW-UHFFFAOYSA-N
<b>Formula:</b>	C13H9ClN2O3
<b>SMILES:</b>	O=C(Nc1ccccc1)c1ccc(Cl)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	276.68
<b>CAS:</b>	41614-16-8

## Physical Properties

Property code	Value	Unit	Source
gf	248.23	kJ/mol	Joback Method
hf	52.86	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.500		Crippen Method
mcvol	187.720	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	853.47	K	Joback Method
tc	1122.75	K	Joback Method
tf	590.27	K	Joback Method
vc	0.720	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.61	J/molxK	853.47	Joback Method
cpg	508.57	J/molxK	898.35	Joback Method
cpg	517.46	J/molxK	943.23	Joback Method
cpg	525.35	J/molxK	988.11	Joback Method
cpg	532.35	J/molxK	1032.99	Joback Method
cpg	538.56	J/molxK	1077.87	Joback Method
cpg	544.05	J/molxK	1122.75	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=C41614168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41614168&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>h vap:</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>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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