

# m-Nitrobenzylidene-p-chlorophenylacetonitrile

<b>Inchi:</b>	InChI=1S/C15H9ClN2O2/c16-14-6-4-12(5-7-14)13(10-17)8-11-2-1-3-15(9-11)18(19)20/h
<b>InchiKey:</b>	RTDWPLYDMXBIEL-MDWZMJQESA-N
<b>Formula:</b>	C15H9ClN2O2
<b>SMILES:</b>	<chem>N#CC(=Cc1cccc([N+](=O)[O-])c1)c1ccc(Cl)cc1</chem>
<b>Mol. weight [g/mol]:</b>	284.70
<b>CAS:</b>	104089-72-7

## Physical Properties

Property code	Value	Unit	Source
gf	509.45	kJ/mol	Joback Method
hf	343.00	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.312		Crippen Method
mcvol	201.430	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	901.31	K	Joback Method
tc	1180.80	K	Joback Method
tf	556.17	K	Joback Method
vc	0.797	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.24	J/molxK	901.31	Joback Method
cpg	540.12	J/molxK	947.89	Joback Method
cpg	549.16	J/molxK	994.47	Joback Method
cpg	557.53	J/molxK	1041.05	Joback Method
cpg	565.35	J/molxK	1087.63	Joback Method
cpg	572.78	J/molxK	1134.22	Joback Method
cpg	579.96	J/molxK	1180.80	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/inchi/InChI%3D1S/C15H9ClN2O2/c16-14-6-4-12(5-7-14)13(10-17">http://webbook.nist.gov/cgi/inchi/InChI%3D1S/C15H9ClN2O2/c16-14-6-4-12(5-7-14)13(10-17</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>
<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>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>m cvol:</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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