

# m-Nitrobenzylidene-2-methylphenylacetonitrile

<b>Inchi:</b>	InChI=1S/C16H12N2O2/c1-12-5-2-3-8-16(12)14(11-17)9-13-6-4-7-15(10-13)18(19)20/h2
<b>InchiKey:</b>	LKSIDQCVROUBOP-NTEUORMPSA-N
<b>Formula:</b>	C16H12N2O2
<b>SMILES:</b>	<chem>Cc1ccccc1C(C#N)=Cc1cccc([N+](=O)[O-])c1</chem>
<b>Mol. weight [g/mol]:</b>	264.28
<b>CAS:</b>	31881-13-7

## Physical Properties

Property code	Value	Unit	Source
chs	-8175.87	kJ/mol	NIST Webbook
chs	-8171.00	kJ/mol	NIST Webbook
gf	529.80	kJ/mol	Joback Method
hf	338.10	kJ/mol	Joback Method
hfs	165.20	kJ/mol	NIST Webbook
hfs	157.00	kJ/mol	NIST Webbook
hfus	36.26	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.967		Crippen Method
mcvol	203.280	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	886.76	K	Joback Method
tc	1159.23	K	Joback Method
tf	537.52	K	Joback Method
vc	0.804	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.68	J/molxK	886.76	Joback Method
cpg	578.13	J/molxK	932.17	Joback Method
cpg	588.63	J/molxK	977.58	Joback Method
cpg	598.33	J/molxK	1022.99	Joback Method
cpg	607.36	J/molxK	1068.40	Joback Method

cpg	615.85	J/mol×K	1113.81	Joback Method
cpg	623.95	J/mol×K	1159.23	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/cbook.cgi?ID=C31881137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31881137&amp;Units=SI</a>
<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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase 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>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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