

# p-Nitrobenzylidene-2,5-dimethylphenylacetonitrile

<b>Inchi:</b>	InChI=1S/C17H14N2O2/c1-12-3-4-13(2)17(9-12)15(11-18)10-14-5-7-16(8-6-14)19(20)21
<b>InchiKey:</b>	KIIBMRYMURXPBD-GDNBJRDFSA-N
<b>Formula:</b>	C17H14N2O2
<b>SMILES:</b>	<chem>Cc1ccc(C)c(C(C#N)=Cc2ccc([N+](=O)[O-])cc2)c1</chem>
<b>Mol. weight [g/mol]:</b>	278.31
<b>CAS:</b>	31881-17-1

## Physical Properties

Property code	Value	Unit	Source
chs	-8847.00	kJ/mol	NIST Webbook
chs	-8842.67	kJ/mol	NIST Webbook
gf	528.59	kJ/mol	Joback Method
hf	305.99	kJ/mol	Joback Method
hfs	153.00	kJ/mol	NIST Webbook
hfs	152.70	kJ/mol	NIST Webbook
hfus	38.46	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.276		Crippen Method
mcvol	217.370	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
tb	914.62	K	Joback Method
tc	1182.06	K	Joback Method
tf	561.31	K	Joback Method
vc	0.861	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.33	J/molxK	914.62	Joback Method
cpg	632.10	J/molxK	959.19	Joback Method
cpg	642.94	J/molxK	1003.77	Joback Method
cpg	652.98	J/molxK	1048.34	Joback Method
cpg	662.34	J/molxK	1092.91	Joback Method

cpg	671.13	J/mol×K	1137.49	Joback Method
cpg	679.48	J/mol×K	1182.06	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C31881171&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31881171&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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