

# Di-o-tolyl-cyano-methane

<b>Inchi:</b>	InChI=1S/C16H15N/c1-12-7-3-5-9-14(12)16(11-17)15-10-6-4-8-13(15)2/h3-10,16H,1-2H
<b>InchiKey:</b>	KDKUNNHFMFKTB-UHFFFAOYSA-N
<b>Formula:</b>	C16H15N
<b>SMILES:</b>	<chem>Cc1cccc1C(C#N)c1cccc1C</chem>
<b>Mol. weight [g/mol]:</b>	221.30
<b>CAS:</b>	116296-33-4

## Physical Properties

Property code	Value	Unit	Source
gf	420.14	kJ/mol	Joback Method
hf	236.15	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	67.18	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.959		Crippen Method
mcvol	190.160	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
tb	730.44	K	Joback Method
tc	978.73	K	Joback Method
tf	397.95	K	Joback Method
vc	0.736	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.06	J/molxK	730.44	Joback Method
cpg	515.93	J/molxK	771.82	Joback Method
cpg	529.61	J/molxK	813.20	Joback Method
cpg	542.19	J/molxK	854.58	Joback Method
cpg	553.73	J/molxK	895.97	Joback Method
cpg	564.31	J/molxK	937.35	Joback Method
cpg	574.01	J/molxK	978.73	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=C116296334&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116296334&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>

# 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>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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