

# Benzeneacetonitrile, 4-methyl-

<b>Other names:</b>	4-Methylbenzyl cyanide p-Xylyl cyanide p-Methylbenzyl cyanide p-Tolylacetonitrile p-Methylphenylacetonitrile 4-Tolylacetonitrile 4-Methylphenylacetonitrile 4-Methylbenzeneacetonitrile
<b>Inchi:</b>	InChI=1S/C9H9N/c1-8-2-4-9(5-3-8)6-7-10/h2-5H,6H2,1H3
<b>InchiKey:</b>	RNHKXHKUKJXLAU-UHFFFAOYSA-N
<b>Formula:</b>	C9H9N
<b>SMILES:</b>	<chem>Cc1ccc(CC#N)cc1</chem>
<b>Mol. weight [g/mol]:</b>	131.17
<b>CAS:</b>	2947-61-7

## Physical Properties

Property code	Value	Unit	Source
gf	260.86	kJ/mol	Joback Method
hf	160.85	kJ/mol	Joback Method
hfus	14.22	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
ie	9.16 ± 0.06	eV	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.061		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	515.70	K	NIST Webbook
tc	767.65	K	Joback Method
tf	295.12	K	Joback Method
vc	0.458	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	243.50	J/mol×K	539.06	Joback Method
cpg	254.71	J/mol×K	577.16	Joback Method
cpg	265.21	J/mol×K	615.26	Joback Method
cpg	275.04	J/mol×K	653.35	Joback Method
cpg	284.23	J/mol×K	691.45	Joback Method
cpg	292.80	J/mol×K	729.55	Joback Method
cpg	300.78	J/mol×K	767.65	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=C2947617&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2947617&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>ie:</b>	Ionization energy
<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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