

3-Methylbenzyl cyanide

Other names:	m-Xylyl cyanide m-Methylbenzyl cyanide m-Tolylacetonitrile m-Methylphenylacetonitrile 3-Tolylacetonitrile 3-Methylphenylacetonitrile Benzeneacetonitrile, 3-methyl- NSC 20695 3-Tolylacetic acid nitrile
Inchi:	InChI=1S/C9H9N/c1-8-3-2-4-9(7-8)5-6-10/h2-4,7H,5H2,1H3
InchiKey:	WOJADIOTNFDWNQ-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	<chem>Cc1cccc(CC#N)c1</chem>
Mol. weight [g/mol]:	131.17
CAS:	2947-60-6

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	9.18 ± 0.04	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	513.70	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
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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2947606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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