Benzeneacetonitrile, 4-methyl-

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

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2947617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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