2-Methylbenzyl cyanide

Other names:	o-Xylyl cyanide
	o-Methylbenzyl cyanide
	o-Tolylacetonitrile
	o-Methylphenylacetonitrile
	2-Tolylacetonitrile
	2-Methylphenylacetonitrile
	Benzeneacetonitrile, 2-methyl-
	Acetonitrile, o-tolyl-
	2-Methylbenzeneacetonitrile
Inchi:	InChI=1S/C9H9N/c1-8-4-2-3-5-9(8)6-7-10/h2-5H,6H2,1H3
InchiKey:	WMGVPDQNPUQRND-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	Cc1ccccc1CC#N
Mol. weight [g/mol]:	131.17
CAS:	22364-68-7

Physical Properties

Property code	Value	Unit	Source
chl	-4921.00	kJ/mol	NIST Webbook
gf	260.86	kJ/mol	Joback Method
hf	160.85	kJ/mol	Joback Method
hfl	92.00	kJ/mol	NIST Webbook
hfus	14.22	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.061		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	485.20	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=C22364687&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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