Benzeneacetonitrile, 4-chloro-

Other names:	Acetonitrile, (p-chlorophenyl)-
	(p-Chlorophenyl)acetonitrile
	(4-Chlorophenyl)acetonitrile
	p-Chlorobenzyl cyanide
	2-(4-Chlorophenyl)acetonitrile
	4-Chlorobenzeneacetonitrile
	4-Chlorobenzyl cyanide
	4-Chlor-benzyl-cyanid
	NSC 49108
Inchi:	InChI=1S/C8H6ClN/c9-8-3-1-7(2-4-8)5-6-10/h1-4H,5H2
InchiKey:	IVYMIRMKXZAHRV-UHFFFAOYSA-N
Formula:	C8H6ClN
SMILES:	N#CCc1ccc(Cl)cc1
Mol. weight [g/mol]:	151.59
CAS:	140-53-4

Physical Properties

Property code	Value	Unit	Source
gf	240.51	kJ/mol	Joback Method
hf	165.75	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
ie	9.43 ± 0.05	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.406		Crippen Method
mcvol	113.440	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	539.20	K	NIST Webbook
tc	791.13	K	Joback Method
tf	313.77	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.76	J/mol×K	553.61	Joback Method
cpg	232.04	J/mol×K	593.20	Joback Method
cpg	240.67	J/mol×K	632.78	Joback Method
cpg	248.68	J/mol×K	672.37	Joback Method
cpg	256.09	J/mol×K	711.95	Joback Method
cpg	262.95	J/mol×K	751.54	Joback Method
cpg	269.27	J/mol×K	791.13	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C140534&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

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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