2-Chlorobenzyl cyanide

Other names:	o-Chlorobenzyl cyanide
	2-Chlorophenylacetonitrile
	o-Chlorophenylacetonitrile
	Benzeneacetonitrile, 2-chloro-
	Acetonitrile, (o-chlorophenyl)-
	2-Chlorobenzeneacetonitrile
Inchi:	InChI=1S/C8H6ClN/c9-8-4-2-1-3-7(8)5-6-10/h1-4H,5H2
InchiKey:	MRDUURPIPLIGQX-UHFFFAOYSA-N
Formula:	C8H6ClN
SMILES:	N#CCc1ccccc1Cl
Mol. weight [g/mol]:	151.59
CAS:	2856-63-5

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
log10ws	-2.83		Crippen Method
logp	2.406		Crippen Method
mcvol	113.440	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1270.00		NIST Webbook
tb	514.20	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

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=C2856635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume