3,4-Dichlorophenylacetonitrile

Other names: 3,4-Dichlorobenzyl cyanide
Benzeneacetonitrile, 3,4-dichloro-
Inchi: InChI=1S/C8H5Cl2N/c9-7-2-1-6(3-4-11)5-8(7)10/h1-2,5H,3H2
InchiKey: QWZNCAFWRZZJMA-UHFFFAOYSA-N
Formula: C8H5Cl2N
SMILES: N#CCc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 186.04
CAS: 3218-49-3

Physical Properties

Property code	Value	Unit	Source
gf	218.95	kJ/mol	Joback Method
hf	138.54	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	56.25	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.059		Crippen Method
mcvol	125.680	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	596.02	K	Joback Method
tc	838.45	K	Joback Method
tf	356.21	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.66	J/mol×K	596.02	Joback Method
cpg	249.88	J/mol×K	636.43	Joback Method
cpg	257.50	J/mol×K	676.83	Joback Method
cpg	264.56	J/mol×K	717.24	Joback Method
cpg	271.08	J/mol×K	757.64	Joback Method
cpg	277.09	J/mol×K	798.05	Joback Method
cpg	282.61	J/mol×K	838.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	1.60	NIST Webbook

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=C3218493&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume