3,4-Dichlorobenzoylacetonitrile

Inchi: InChI=1S/C9H5Cl2NO/c10-7-2-1-6(5-8(7)11)9(13)3-4-12/h1-2,5H,3H2
InchiKey: HUEULXLHYYYTTP-UHFFFAOYSA-N
Formula: C9H5Cl2NO
SMILES: N#CCC(=O)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 214.05
CAS: 4640-68-0

Physical Properties

Property code	Value	Unit	Source
gf	98.45	kJ/mol	Joback Method
hf	5.32	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.090		Crippen Method
mcvol	141.340	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	672.77	K	Joback Method
tc	916.39	K	Joback Method
tf	417.41	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.00	J/mol×K	672.77	Joback Method
cpg	301.02	J/mol×K	713.37	Joback Method
cpg	308.40	J/mol×K	753.98	Joback Method
cpg	315.17	J/mol×K	794.58	Joback Method
cpg	321.35	J/mol×K	835.19	Joback Method
cpg	326.98	J/mol×K	875.79	Joback Method
cpg	332.09	J/mol×K	916.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4640680&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
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