3-Chlorobenzoylacetonitrile

Inchi: InChI=1S/C9H6ClNO/c10-8-3-1-2-7(6-8)9(12)4-5-11/h1-3,6H,4H2
InchiKey: IUDFNNHFARLIPF-UHFFFAOYSA-N
Formula: C9H6ClNO
SMILES: N#CCC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 179.60
CAS: 21667-62-9

Physical Properties

Property code	Value	Unit	Source
gf	120.01	kJ/mol	Joback Method
hf	32.53	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	60.18	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.436		Crippen Method
mcvol	129.100	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	630.36	K	Joback Method
tc	870.27	K	Joback Method
tf	374.97	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.38	J/mol×K	630.36	Joback Method
cpg	284.47	J/mol×K	670.34	Joback Method
cpg	292.85	J/mol×K	710.33	Joback Method
cpg	300.57	J/mol×K	750.31	Joback Method
cpg	307.66	J/mol×K	790.30	Joback Method
cpg	314.15	J/mol×K	830.28	Joback Method
cpg	320.08	J/mol×K	870.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21667629&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