2,4,6-Trichlorobenzonitrile

Inchi: InChI=1S/C7H2Cl3N/c8-4-1-6(9)5(3-11)7(10)2-4/h1-2H
InchiKey: PGODHCIOIPODFE-UHFFFAOYSA-N
Formula: C7H2Cl3N
SMILES: N#Cc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 206.46
CAS: 6575-05-9

Physical Properties

Property code	Value	Unit	Source
gf	188.97	kJ/mol	Joback Method
hf	131.97	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	59.07	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.518		Crippen Method
mcvol	123.830	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	615.55	K	Joback Method
tc	867.76	K	Joback Method
tf	387.38	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.69	J/mol×K	615.55	Joback Method
cpg	220.70	J/mol×K	657.59	Joback Method
cpg	226.25	J/mol×K	699.62	Joback Method
cpg	231.35	J/mol×K	741.66	Joback Method
cpg	236.03	J/mol×K	783.69	Joback Method
cpg	240.30	J/mol×K	825.73	Joback Method
cpg	244.19	J/mol×K	867.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6575059&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