Dichloroacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C9H5Cl2NO2/c10-8(11)9(13)14-7-3-1-6(5-12)2-4-7/h1-4,8H
InchiKey: FZXOVVSGYFFISB-UHFFFAOYSA-N
Formula: C9H5Cl2NO2
SMILES: N#Cc1ccc(OC(=O)C(Cl)Cl)cc1
Mol. weight [g/mol]: 230.05

Physical Properties

Property code	Value	Unit	Source
gf	0.64	kJ/mol	Joback Method
hf	-120.71	kJ/mol	Joback Method
hfus	21.88	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.267		Crippen Method
mcvol	147.210	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1593.00		NIST Webbook
tb	689.77	K	Joback Method
tc	933.64	K	Joback Method
tf	412.12	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.89	J/mol×K	689.77	Joback Method
cpg	325.22	J/mol×K	730.41	Joback Method
cpg	332.84	J/mol×K	771.06	Joback Method
cpg	339.75	J/mol×K	811.70	Joback Method
cpg	345.98	J/mol×K	852.35	Joback Method
cpg	351.55	J/mol×K	892.99	Joback Method
cpg	356.47	J/mol×K	933.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307587&Units=SI

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