Chloroacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C9H6ClNO2/c10-5-9(12)13-8-3-1-7(6-11)2-4-8/h1-4H,5H2
InchiKey: APQLVUNYVFVTPC-UHFFFAOYSA-N
Formula: C9H6ClNO2
SMILES: N#Cc1ccc(OC(=O)CCl)cc1
Mol. weight [g/mol]: 195.60

Physical Properties

Property code	Value	Unit	Source
gf	15.01	kJ/mol	Joback Method
hf	-99.69	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.702		Crippen Method
mcvol	134.970	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
tb	652.78	K	Joback Method
tc	889.03	K	Joback Method
tf	397.20	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.86	J/mol×K	652.78	Joback Method
cpg	305.89	J/mol×K	692.15	Joback Method
cpg	314.24	J/mol×K	731.53	Joback Method
cpg	321.94	J/mol×K	770.90	Joback Method
cpg	328.99	J/mol×K	810.28	Joback Method
cpg	335.41	J/mol×K	849.65	Joback Method
cpg	341.22	J/mol×K	889.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307715&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume