Carbonic acid, 2-chloroethyl 4-cyanophenyl ester

Inchi: InChI=1S/C10H8ClNO3/c11-5-6-14-10(13)15-9-3-1-8(7-12)2-4-9/h1-4H,5-6H2
InchiKey: YWQMXAKUZKIOQC-UHFFFAOYSA-N
Formula: C10H8ClNO3
SMILES: N#Cc1ccc(OC(=O)OCCCl)cc1
Mol. weight [g/mol]: 225.63

Physical Properties

Property code	Value	Unit	Source
gf	-81.57	kJ/mol	Joback Method
hf	-252.55	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.312		Crippen Method
mcvol	154.930	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1818.00		NIST Webbook
tb	698.08	K	Joback Method
tc	926.45	K	Joback Method
tf	430.70	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.97	J/mol×K	698.08	Joback Method
cpg	376.74	J/mol×K	736.14	Joback Method
cpg	385.78	J/mol×K	774.20	Joback Method
cpg	394.10	J/mol×K	812.26	Joback Method
cpg	401.70	J/mol×K	850.32	Joback Method
cpg	408.56	J/mol×K	888.38	Joback Method
cpg	414.69	J/mol×K	926.45	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=U357888&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