Carbonic acid, 2-chloroethyl 4-nitrophenyl ester

Inchi: InChI=1S/C9H8ClNO5/c10-5-6-15-9(12)16-8-3-1-7(2-4-8)11(13)14/h1-4H,5-6H2
InchiKey: XTINYHMDVMSXCV-UHFFFAOYSA-N
Formula: C9H8ClNO5
SMILES: O=C(OCCCl)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 245.62

Physical Properties

Property code	Value	Unit	Source
gf	-187.62	kJ/mol	Joback Method
hf	-407.55	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.349		Crippen Method
mcvol	156.880	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	1931.00		NIST Webbook
tb	724.96	K	Joback Method
tc	965.97	K	Joback Method
tf	498.05	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.27	J/mol×K	724.96	Joback Method
cpg	400.48	J/mol×K	765.13	Joback Method
cpg	409.80	J/mol×K	805.30	Joback Method
cpg	418.25	J/mol×K	845.46	Joback Method
cpg	425.82	J/mol×K	885.63	Joback Method
cpg	432.51	J/mol×K	925.80	Joback Method
cpg	438.34	J/mol×K	965.97	Joback Method

Sources

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=U357890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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