Carbonic acid, 2-chloroethyl 4-chlorophenyl ester

Inchi: InChI=1S/C9H8Cl2O3/c10-5-6-13-9(12)14-8-3-1-7(11)2-4-8/h1-4H,5-6H2

InchiKey: UGCFAIRGFNSYNZ-UHFFFAOYSA-N

Formula: C9H8Cl2O3

SMILES: O=C(OCCCl)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 235.06

Physical Properties

Property code	Value	Unit	Source
gf	-235.10	kJ/mol	Joback Method
hf	-412.53	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	58.90	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.094		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1666.00		NIST Webbook
tb	610.55	K	Joback Method
tc	833.74	K	Joback Method
tf	384.36	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.41	J/mol×K	610.55	Joback Method
cpg	337.02	J/mol×K	647.75	Joback Method
cpg	346.97	J/mol×K	684.95	Joback Method
cpg	356.26	J/mol×K	722.15	Joback Method
cpg	364.89	J/mol×K	759.35	Joback Method
cpg	372.86	J/mol×K	796.54	Joback Method
cpg	380.16	J/mol×K	833.74	Joback Method
dvisc	0.0011817	Pa×s	384.36	Joback Method
dvisc	0.0007471	Pa×s	422.06	Joback Method

dvisc	0.0005092	Pa×s	459.76	Joback Method
dvisc	0.0003678	Pa×s	497.45	Joback Method
dvisc	0.0002782	Pa×s	535.15	Joback Method
dvisc	0.0002182	Pa×s	572.85	Joback Method
dvisc	0.0001764	Pa×s	610.55	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=U357885&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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