Carbonic acid, 2-chloroethyl 3,4-dichlorophenyl ester

Inchi: InChI=1S/C9H7Cl3O3/c10-3-4-14-9(13)15-6-1-2-7(11)8(12)5-6/h1-2,5H,3-4H2

InchiKey: YLLLCCMOLMFOGA-UHFFFAOYSA-N

Formula: C9H7Cl3O3

SMILES: O=C(OCCCl)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 269.51

Physical Properties

Property code	Value	Unit	Source
gf	-256.66	kJ/mol	Joback Method
hf	-439.74	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	63.95	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.748		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1852.00		NIST Webbook
tb	652.96	K	Joback Method
tc	880.39	K	Joback Method
tf	426.80	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.70	J/mol×K	652.96	Joback Method
cpg	356.30	J/mol×K	690.86	Joback Method
cpg	365.25	J/mol×K	728.77	Joback Method
cpg	373.55	J/mol×K	766.67	Joback Method
cpg	381.19	J/mol×K	804.58	Joback Method
cpg	388.17	J/mol×K	842.48	Joback Method
cpg	394.47	J/mol×K	880.39	Joback Method
dvisc	0.0008821	Pa×s	426.80	Joback Method
dvisc	0.0005925	Pa×s	464.49	Joback Method

dvisc	0.0004225	Pa×s	502.19	Joback Method
dvisc	0.0003158	Pa×s	539.88	Joback Method
dvisc	0.0002452	Pa×s	577.57	Joback Method
dvisc	0.0001964	Pa×s	615.27	Joback Method
dvisc	0.0001614	Pa×s	652.96	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=U357889&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