Ethyl 2,4,5-trichlorophenyl carbonate

Inchi: InChI=1S/C9H7Cl3O3/c1-2-14-9(13)15-8-4-6(11)5(10)3-7(8)12/h3-4H,2H2,1H3
InchiKey: GPVCBFIVLNSTRS-UHFFFAOYSA-N
Formula: C9H7Cl3O3
SMILES: CCOC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 269.51
CAS: 22876-29-5

Physical Properties

Property code	Value	Unit	Source
gf	-266.29	kJ/mol	Joback Method
hf	-451.21	kJ/mol	Joback Method
hfus	28.51	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.182		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	657.94	K	Joback Method
tc	886.25	K	Joback Method
tf	439.32	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.09	J/mol×K	657.94	Joback Method
cpg	354.53	J/mol×K	695.99	Joback Method
cpg	363.36	J/mol×K	734.04	Joback Method
cpg	371.56	J/mol×K	772.10	Joback Method
cpg	379.13	J/mol×K	810.15	Joback Method
cpg	386.04	J/mol×K	848.20	Joback Method
cpg	392.29	J/mol×K	886.25	Joback Method
dvisc	0.0007498	Pa×s	439.32	Joback Method
dvisc	0.0005253	Pa×s	475.76	Joback Method

dvisc	0.0003871	Pa×s	512.19	Joback Method
dvisc	0.0002970	Pa×s	548.63	Joback Method
dvisc	0.0002356	Pa×s	585.07	Joback Method
dvisc	0.0001920	Pa×s	621.50	Joback Method
dvisc	0.0001601	Pa×s	657.94	Joback Method

Sources

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=C22876295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume