3-(2,4,5-Trichlorophenoxy)-1,2-propanediol bis-(2,2-dichloropropionate)

Inchi: InChI=1S/C15H13Cl7O5/c1-14(19,20)12(23)26-6-7(27-13(24)15(2,21)22)5-25-11-4-9(17)
InchiKey: KKLFMUOVHGJHOX-UHFFFAOYSA-N
Formula: C15H13Cl7O5
SMILES: CC(Cl)(Cl)C(=O)OCC(COc1cc(Cl)c(Cl)cc1Cl)OC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]: 521.43
CAS: 101096-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-494.17	kJ/mol	Joback Method
hf	-905.59	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	101.68	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.868		Crippen Method
mcvol	304.880	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
tb	1014.33	K	Joback Method
tc	1261.62	K	Joback Method
tf	688.62	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.88	J/mol×K	1014.33	Joback Method
cpg	769.15	J/mol×K	1055.54	Joback Method
cpg	774.44	J/mol×K	1096.76	Joback Method
cpg	778.79	J/mol×K	1137.97	Joback Method
cpg	782.26	J/mol×K	1179.19	Joback Method
cpg	784.93	J/mol×K	1220.40	Joback Method
cpg	786.84	J/mol×K	1261.62	Joback Method
dvisc	0.0000987	Pa×s	688.62	Joback Method
dvisc	0.0000633	Pa×s	742.90	Joback Method

dvisc	0.0000432	Pa×s	797.19	Joback Method
dvisc	0.0000309	Pa×s	851.48	Joback Method
dvisc	0.0000230	Pa×s	905.76	Joback Method
dvisc	0.0000177	Pa×s	960.05	Joback Method
dvisc	0.0000141	Pa×s	1014.33	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=C101096600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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