Succinic acid, 2,2-dichloroethyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C12H9Cl5O4/c13-6-3-8(15)9(4-7(6)14)21-12(19)2-1-11(18)20-5-10(16)17/h3-4
InchiKey: ZEHHYZPDYYOUNR-UHFFFAOYSA-N
Formula: C12H9Cl5O4
SMILES: O=C(CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)OCC(Cl)Cl
Mol. weight [g/mol]: 394.46

Physical Properties

Property code	Value	Unit	Source
gf	-396.25	kJ/mol	Joback Method
hf	-662.47	kJ/mol	Joback Method
hfus	42.75	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.679		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook
tb	854.87	K	Joback Method
tc	1086.74	K	Joback Method
tf	567.90	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.11	J/mol×K	854.87	Joback Method
cpg	550.19	J/mol×K	893.52	Joback Method
cpg	557.35	J/mol×K	932.16	Joback Method
cpg	563.59	J/mol×K	970.81	Joback Method
cpg	568.92	J/mol×K	1009.45	Joback Method
cpg	573.33	J/mol×K	1048.10	Joback Method
cpg	576.82	J/mol×K	1086.74	Joback Method
dvisc	0.0004367	Pa×s	567.90	Joback Method

dvisc	0.0002917	Pa×s	615.73	Joback Method
dvisc	0.0002065	Pa×s	663.56	Joback Method
dvisc	0.0001531	Pa×s	711.38	Joback Method
dvisc	0.0001179	Pa×s	759.21	Joback Method
dvisc	0.0000937	Pa×s	807.04	Joback Method
dvisc	0.0000763	Pa×s	854.87	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=U389964&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume