Succinic acid, 2,4,6-trichlorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H25Cl3O4/c1-20(2,3)12-4-6-14(7-5-12)26-17(24)8-9-18(25)27-19-15(22)10
InchiKey: LWEKSCLFWMHMFX-UHFFFAOYSA-N
Formula: C20H25Cl3O4
SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)Oc2c(Cl)cc(Cl)cc2Cl)CC1
Mol. weight [g/mol]: 435.77

Physical Properties

Property code	Value	Unit	Source
gf	-283.01	kJ/mol	Joback Method
hf	-765.60	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	94.67	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.481		Crippen Method
mcvol	309.640	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	975.14	K	Joback Method
tc	1214.05	K	Joback Method
tf	618.78	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.54	J/mol×K	975.14	Joback Method
cpg	961.07	J/mol×K	1014.96	Joback Method
cpg	972.02	J/mol×K	1054.78	Joback Method
cpg	981.45	J/mol×K	1094.60	Joback Method
cpg	989.39	J/mol×K	1134.42	Joback Method
cpg	995.91	J/mol×K	1174.23	Joback Method
cpg	1001.05	J/mol×K	1214.05	Joback Method
dvisc	0.0002824	Pa×s	618.78	Joback Method

dvisc	0.0001735	Pa×s	678.17	Joback Method
dvisc	0.0001153	Pa×s	737.57	Joback Method
dvisc	0.0000815	Pa×s	796.96	Joback Method
dvisc	0.0000604	Pa×s	856.35	Joback Method
dvisc	0.0000465	Pa×s	915.75	Joback Method
dvisc	0.0000370	Pa×s	975.14	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=U390204&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