Succinic acid, 2,3-dichlorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H26Cl2O4/c1-20(2,3)13-7-9-14(10-8-13)25-17(23)11-12-18(24)26-16-6-4-5

InchiKey: HYMITNDSJTYLJT-UHFFFAOYSA-N

Formula: C20H26Cl2O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)CC1

Mol. weight [g/mol]: 401.32

Physical Properties

Property code	Value	Unit	Source
gf	-261.45	kJ/mol	Joback Method
hf	-738.39	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	89.62	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.827		Crippen Method
mcvol	297.400	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2948.00		NIST Webbook
rinpol	2948.00		NIST Webbook
tb	932.73	K	Joback Method
tc	1167.28	K	Joback Method
tf	576.34	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.70	J/mol×K	932.73	Joback Method
cpg	942.00	J/mol×K	971.82	Joback Method
cpg	954.72	J/mol×K	1010.91	Joback Method
cpg	965.92	J/mol×K	1050.00	Joback Method
cpg	975.66	J/mol×K	1089.10	Joback Method
cpg	983.98	J/mol×K	1128.19	Joback Method
cpg	990.94	J/mol×K	1167.28	Joback Method
dvisc	0.0003885	Pa×s	576.34	Joback Method

dvisc	0.0002268	Pa×s	635.74	Joback Method
dvisc	0.0001451	Pa×s	695.14	Joback Method
dvisc	0.0000996	Pa×s	754.53	Joback Method
dvisc	0.0000723	Pa×s	813.93	Joback Method
dvisc	0.0000548	Pa×s	873.33	Joback Method
dvisc	0.0000430	Pa×s	932.73	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=U390203&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