Succinic acid, 3-chlorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H27ClO4/c1-20(2,3)14-7-9-16(10-8-14)24-18(22)11-12-19(23)25-17-6-4-5-

InchiKey: RSGWHPZRRSBHEZ-UHFFFAOYSA-N

Formula: C20H27ClO4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)Oc2cccc(Cl)c2)CC1

Mol. weight [g/mol]: 366.88

Physical Properties

Property code	Value	Unit	Source
gf	-239.89	kJ/mol	Joback Method
hf	-711.18	kJ/mol	Joback Method
hfus	36.47	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.174		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	890.32	K	Joback Method
tc	1120.79	K	Joback Method
tf	533.90	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.34	J/mol×K	890.32	Joback Method
cpg	920.41	J/mol×K	928.73	Joback Method
cpg	934.91	J/mol×K	967.14	Joback Method
cpg	947.88	J/mol×K	1005.56	Joback Method
cpg	959.37	J/mol×K	1043.97	Joback Method
cpg	969.46	J/mol×K	1082.38	Joback Method
cpg	978.18	J/mol×K	1120.79	Joback Method
dvisc	0.0005477	Pa×s	533.90	Joback Method

dvisc	0.0003005	Pa×s	593.30	Joback Method
dvisc	0.0001839	Pa×s	652.71	Joback Method
dvisc	0.0001222	Pa×s	712.11	Joback Method
dvisc	0.0000864	Pa×s	771.51	Joback Method
dvisc	0.0000642	Pa×s	830.92	Joback Method
dvisc	0.0000497	Pa×s	890.32	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=U390202&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