Succinic acid, hept-2-yl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C21H38O4/c1-6-7-8-9-16(2)24-19(22)14-15-20(23)25-18-12-10-17(11-13-18)2

InchiKey: VJIKFHOGRCJRAK-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OC1CCC(C(C)(C)C)CC1

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-324.76	kJ/mol	Joback Method
hf	-946.42	kJ/mol	Joback Method
hfus	37.69	kJ/mol	Joback Method
hvap	79.09	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.427		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1154.57	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	843.67	K	Joback Method
tc	1046.08	K	Joback Method
tf	461.31	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.02	J/mol×K	843.67	Joback Method
cpg	1116.56	J/mol×K	1012.35	Joback Method
cpg	1102.36	J/mol×K	978.61	Joback Method
cpg	1086.85	J/mol×K	944.88	Joback Method
cpg	1069.98	J/mol×K	911.14	Joback Method
cpg	1051.71	J/mol×K	877.41	Joback Method
cpg	1129.48	J/mol×K	1046.08	Joback Method
dvisc	0.0000445	Pa×s	843.67	Joback Method

dvisc	0.0000606	Pa×s	779.94	Joback Method
dvisc	0.0000870	Pa×s	716.22	Joback Method
dvisc	0.0001343	Pa×s	652.49	Joback Method
dvisc	0.0002275	Pa×s	588.76	Joback Method
dvisc	0.0004382	Pa×s	525.04	Joback Method
dvisc	0.0010115	Pa×s	461.31	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=U390189&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume