Succinic acid, cis-4-tert-butylcyclohexyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C24H42O4/c1-23(2,3)17-7-11-19(12-8-17)27-21(25)15-16-22(26)28-20-13-9-1

InchiKey: IJKKIWACMLFLBE-UHFFFAOYSA-N

Formula: C24H42O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)OC2CCC(C(C)(C)C)CC2)CC1

Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-277.48	kJ/mol	Joback Method
hf	-977.83	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	84.98	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.063		Crippen Method
mcvol	342.180	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	924.40	K	Joback Method
tc	1148.21	K	Joback Method
tf	515.68	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.56	J/mol×K	924.40	Joback Method
cpg	1239.98	J/mol×K	961.70	Joback Method
cpg	1258.48	J/mol×K	999.00	Joback Method
cpg	1275.16	J/mol×K	1036.31	Joback Method
cpg	1290.08	J/mol×K	1073.61	Joback Method
cpg	1303.33	J/mol×K	1110.91	Joback Method
cpg	1314.98	J/mol×K	1148.21	Joback Method
dvisc	0.0006706	Pa×s	515.68	Joback Method

dvisc	0.0003009	Pa×s	583.80	Joback Method
dvisc	0.0001597	Pa×s	651.92	Joback Method
dvisc	0.0000955	Pa×s	720.04	Joback Method
dvisc	0.0000624	Pa×s	788.16	Joback Method
dvisc	0.0000437	Pa×s	856.28	Joback Method
dvisc	0.0000322	Pa×s	924.40	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=U390207&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