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

Inchi: InChI=1S/C21H36O4/c1-21(2,3)17-9-11-18(12-10-17)25-20(23)14-13-19(22)24-15-16-7-5

InchiKey: QPYDTLBLTZOHGN-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)OCC2CCCCC2)CC1

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-297.87	kJ/mol	Joback Method
hf	-886.82	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	79.91	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.038		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1083.59	K	Joback Method
tf	483.69	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.74	J/mol×K	863.66	Joback Method
cpg	1049.24	J/mol×K	900.31	Joback Method
cpg	1067.94	J/mol×K	936.97	Joback Method
cpg	1084.90	J/mol×K	973.62	Joback Method
cpg	1100.17	J/mol×K	1010.28	Joback Method
cpg	1113.79	J/mol×K	1046.93	Joback Method
cpg	1125.83	J/mol×K	1083.59	Joback Method
dvisc	0.0009749	Pa×s	483.69	Joback Method

dvisc	0.0004462	Pa×s	547.02	Joback Method
dvisc	0.0002401	Pa×s	610.35	Joback Method
dvisc	0.0001452	Pa×s	673.68	Joback Method
dvisc	0.0000957	Pa×s	737.00	Joback Method
dvisc	0.0000674	Pa×s	800.33	Joback Method
dvisc	0.0000500	Pa×s	863.66	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=U390191&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

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