Succinic acid, 3-methylbut-2-yl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C19H34O4/c1-13(2)14(3)22-17(20)11-12-18(21)23-16-9-7-15(8-10-16)19(4,5)6

InchiKey: YRCWXOLGCPYLKU-UHFFFAOYSA-N

Formula: C19H34O4

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

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-344.04	kJ/mol	Joback Method
hf	-910.42	kJ/mol	Joback Method
hfus	28.99	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.502		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	797.47	K	Joback Method
tc	1002.71	K	Joback Method
tf	423.77	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.83	J/mol×K	797.47	Joback Method
cpg	996.69	J/mol×K	968.50	Joback Method
cpg	982.22	J/mol×K	934.30	Joback Method
cpg	966.43	J/mol×K	900.09	Joback Method
cpg	949.29	J/mol×K	865.88	Joback Method
cpg	930.77	J/mol×K	831.68	Joback Method
cpg	1009.87	J/mol×K	1002.71	Joback Method
dvisc	0.0000550	Pa×s	797.47	Joback Method

dvisc	0.0000758	Pa×s	735.19	Joback Method
dvisc	0.0001110	Pa×s	672.90	Joback Method
dvisc	0.0001758	Pa×s	610.62	Joback Method
dvisc	0.0003087	Pa×s	548.34	Joback Method
dvisc	0.0006266	Pa×s	486.05	Joback Method
dvisc	0.0015658	Pa×s	423.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390196&Units=SI
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

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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