

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/molxK	797.47	Joback Method
cpg	996.69	J/molxK	968.50	Joback Method
cpg	982.22	J/molxK	934.30	Joback Method
cpg	966.43	J/molxK	900.09	Joback Method
cpg	949.29	J/molxK	865.88	Joback Method
cpg	930.77	J/molxK	831.68	Joback Method
cpg	1009.87	J/molxK	1002.71	Joback Method
dvisc	0.0000550	Paxs	797.47	Joback Method

dvisc	0.0000758	Paxs	735.19	Joback Method
dvisc	0.0001110	Paxs	672.90	Joback Method
dvisc	0.0001758	Paxs	610.62	Joback Method
dvisc	0.0003087	Paxs	548.34	Joback Method
dvisc	0.0006266	Paxs	486.05	Joback Method
dvisc	0.0015658	Paxs	423.77	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=U390196&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

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