

Succinic acid, hept-2-yl trans-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:	CCCCC(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
mvol	310.770	ml/mol	McGowan Method
pc	1154.57	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	843.67	K	Joback Method
tc	1046.08	K	Joback Method
tf	461.31	K	Joback Method
vc	1.175	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.02	J/molxK	843.67	Joback Method
cpg	1051.71	J/molxK	877.41	Joback Method
cpg	1069.98	J/molxK	911.14	Joback Method
cpg	1086.85	J/molxK	944.88	Joback Method
cpg	1102.36	J/molxK	978.61	Joback Method
cpg	1116.56	J/molxK	1012.35	Joback Method
cpg	1129.48	J/molxK	1046.08	Joback Method
dvisc	0.0010115	Paxs	461.31	Joback Method

dvisc	0.0004382	Paxs	525.04	Joback Method
dvisc	0.0002275	Paxs	588.76	Joback Method
dvisc	0.0001343	Paxs	652.49	Joback Method
dvisc	0.0000870	Paxs	716.22	Joback Method
dvisc	0.0000606	Paxs	779.94	Joback Method
dvisc	0.0000445	Paxs	843.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390199&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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