

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

Inchi: InChI=1S/C20H36O4/c1-7-17(14(2)3)24-19(22)13-12-18(21)23-16-10-8-15(9-11-16)20(4)
InchiKey: LXOLVIFTJKSYDM-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: CCC(OC(=O)CCC(=O)OC1CCC(C(C)(C)C)CC1)C(C)C
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-335.62	kJ/mol	Joback Method
hf	-931.06	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	76.47	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.893		Crippen Method
mvol	296.680	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	820.35	K	Joback Method
tc	1024.80	K	Joback Method
tf	435.04	K	Joback Method
vc	1.113	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.31	J/molxK	820.35	Joback Method
cpg	1056.78	J/molxK	990.72	Joback Method
cpg	1042.42	J/molxK	956.65	Joback Method
cpg	1026.74	J/molxK	922.57	Joback Method
cpg	1009.68	J/molxK	888.50	Joback Method
cpg	991.21	J/molxK	854.42	Joback Method
cpg	1069.84	J/molxK	1024.80	Joback Method
dvisc	0.0000474	Paxs	820.35	Joback Method

dvisc	0.0000655	Paxs	756.13	Joback Method
dvisc	0.0000961	Paxs	691.91	Joback Method
dvisc	0.0001525	Paxs	627.69	Joback Method
dvisc	0.0002689	Paxs	563.48	Joback Method
dvisc	0.0005485	Paxs	499.26	Joback Method
dvisc	0.0013809	Paxs	435.04	Joback Method

Sources

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=U390197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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