Glutaric acid, 3-methylbut-2-yl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H36O4/c1-14(2)15(3)23-18(21)8-7-9-19(22)24-17-12-10-16(11-13-17)20(4

InchiKey: DQHCKUBYXFRJAB-UHFFFAOYSA-N

Formula: C20H36O4

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

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
mcvol	296.680	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	820.35	K	Joback Method
tc	1024.80	K	Joback Method
tf	435.04	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.31	J/mol×K	820.35	Joback Method
cpg	991.21	J/mol×K	854.42	Joback Method
cpg	1009.68	J/mol×K	888.50	Joback Method
cpg	1026.74	J/mol×K	922.57	Joback Method
cpg	1042.42	J/mol×K	956.65	Joback Method
cpg	1056.78	J/mol×K	990.72	Joback Method
cpg	1069.84	J/mol×K	1024.80	Joback Method
dvisc	0.0013809	Pa×s	435.04	Joback Method

dvisc	0.0005485	Pa×s	499.26	Joback Method
dvisc	0.0002689	Pa×s	563.48	Joback Method
dvisc	0.0001525	Pa×s	627.69	Joback Method
dvisc	0.0000961	Pa×s	691.91	Joback Method
dvisc	0.0000655	Pa×s	756.13	Joback Method
dvisc	0.0000474	Pa×s	820.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393385&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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