Glutaric acid, dodec-2-en-1-yl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C27H48O4/c1-5-6-7-8-9-10-11-12-13-14-22-30-25(28)16-15-17-26(29)31-24-2

InchiKey: DNDDXYCKEPNEAX-YPKPFQOOSA-N

Formula: C27H48O4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)OC1CCC(C(C)(C)C)CC1

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-191.58	kJ/mol	Joback Method
hf	-947.76	kJ/mol	Joback Method
hfus	56.95	kJ/mol	Joback Method
hvap	92.79	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.545		Crippen Method
mcvol	391.010	ml/mol	McGowan Method
pc	828.11	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	985.55	K	Joback Method
tc	1206.67	K	Joback Method
tf	538.85	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.96	J/mol×K	985.55	Joback Method
cpg	1465.84	J/mol×K	1169.81	Joback Method
cpg	1451.97	J/mol×K	1132.96	Joback Method
cpg	1436.74	J/mol×K	1096.11	Joback Method
cpg	1420.05	J/mol×K	1059.26	Joback Method
cpg	1401.81	J/mol×K	1022.40	Joback Method
cpg	1478.42	J/mol×K	1206.67	Joback Method
dvisc	0.0000169	Pa×s	985.55	Joback Method

dvisc	0.0000229	Pa×s	911.10	Joback Method
dvisc	0.0000328	Pa×s	836.65	Joback Method
dvisc	0.0000505	Pa×s	762.20	Joback Method
dvisc	0.0000851	Pa×s	687.75	Joback Method
dvisc	0.0001631	Pa×s	613.30	Joback Method
dvisc	0.0003739	Pa×s	538.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393392&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