Glutaric acid, hept-2-yl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C22H40O4/c1-6-7-8-10-17(2)25-20(23)11-9-12-21(24)26-19-15-13-18(14-16-1

InchiKey: BYBZFAUTJXZQBV-UHFFFAOYSA-N

Formula: C22H40O4

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

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-316.34	kJ/mol	Joback Method
hf	-967.06	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	81.31	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.817		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1082.78	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	866.55	K	Joback Method
tc	1069.84	K	Joback Method
tf	472.58	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.84	J/mol×K	866.55	Joback Method
cpg	1113.55	J/mol×K	900.43	Joback Method
cpg	1131.78	J/mol×K	934.31	Joback Method
cpg	1148.59	J/mol×K	968.19	Joback Method
cpg	1164.01	J/mol×K	1002.07	Joback Method
cpg	1178.09	J/mol×K	1035.96	Joback Method
cpg	1190.86	J/mol×K	1069.84	Joback Method
dvisc	0.0008924	Pa×s	472.58	Joback Method

dvisc	0.0003833	Pa×s	538.24	Joback Method
dvisc	0.0001979	Pa×s	603.90	Joback Method
dvisc	0.0001163	Pa×s	669.56	Joback Method
dvisc	0.0000751	Pa×s	735.23	Joback Method
dvisc	0.0000522	Pa×s	800.89	Joback Method
dvisc	0.0000383	Pa×s	866.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393403&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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