Glutaric acid, cyclohexylmethyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C22H38O4/c1-22(2,3)18-12-14-19(15-13-18)26-21(24)11-7-10-20(23)25-16-17

InchiKey: DEMOISFIAXGSHO-UHFFFAOYSA-N

Formula: C22H38O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)OCC2CCCCC2)CC1

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-289.45	kJ/mol	Joback Method
hf	-907.46	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	82.13	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.428		Crippen Method
mcvol	314.000	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1105.42	K	Joback Method
tf	494.96	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.60	J/mol×K	886.54	Joback Method
cpg	1110.82	J/mol×K	923.02	Joback Method
cpg	1129.24	J/mol×K	959.50	Joback Method
cpg	1145.91	J/mol×K	995.98	Joback Method
cpg	1160.89	J/mol×K	1032.46	Joback Method
cpg	1174.22	J/mol×K	1068.94	Joback Method
cpg	1185.97	J/mol×K	1105.42	Joback Method
dvisc	0.0008617	Pa×s	494.96	Joback Method

dvisc	0.0003908	Pa×s	560.22	Joback Method
dvisc	0.0002090	Pa×s	625.49	Joback Method
dvisc	0.0001258	Pa×s	690.75	Joback Method
dvisc	0.0000827	Pa×s	756.01	Joback Method
dvisc	0.0000581	Pa×s	821.28	Joback Method
dvisc	0.0000430	Pa×s	886.54	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=U393404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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