Glutaric acid, isohexyl 2-tert-butyl-6-methylphenyl ester

Inchi: InChI=1S/C22H34O4/c1-16(2)10-9-15-25-19(23)13-8-14-20(24)26-21-17(3)11-7-12-18(2

InchiKey: CYXKAPIEUFSXRI-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: Cc1cccc(C(C)(C)C)c1OC(=O)CCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-239.93	kJ/mol	Joback Method
hf	-787.45	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.348		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	2520.00		NIST Webbook
tb	888.31	K	Joback Method
tc	1097.09	K	Joback Method
tf	520.90	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.71	J/mol×K	888.31	Joback Method
cpg	1014.35	J/mol×K	923.11	Joback Method
cpg	1029.75	J/mol×K	957.90	Joback Method
cpg	1043.94	J/mol×K	992.70	Joback Method
cpg	1056.97	J/mol×K	1027.49	Joback Method
cpg	1068.88	J/mol×K	1062.29	Joback Method
cpg	1079.71	J/mol×K	1097.09	Joback Method
dvisc	0.0004195	Pa×s	520.90	Joback Method
dvisc	0.0002142	Pa×s	582.13	Joback Method

dvisc	0.0001243	Pa×s	643.37	Joback Method
dvisc	0.0000793	Pa×s	704.61	Joback Method
dvisc	0.0000544	Pa×s	765.84	Joback Method
dvisc	0.0000394	Pa×s	827.07	Joback Method
dvisc	0.0000299	Pa×s	888.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359136&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