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

Inchi: InChI=1S/C25H44O4/c1-24(2,3)18-10-14-20(15-11-18)28-22(26)8-7-9-23(27)29-21-16-12-19(13-17-21)25(4,5)6/h18-21H,7-17H2,1-6H3/t18-,19-,20+,21+

InchiKey: LLRPKUOCTIYRIM-UHFFFAOYSA-N

Formula: C25H44O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)OC2CCC(C(C)(C)C)CC2)CC1

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-269.06	kJ/mol	Joback Method
hf	-998.47	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.453		Crippen Method
mcvol	356.270	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2872.00		NIST Webbook
rinpol	2872.00		NIST Webbook
tb	947.28	K	Joback Method
tc	1171.20	K	Joback Method
tf	526.95	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.70	J/mol×K	947.28	Joback Method
cpg	1302.81	J/mol×K	984.60	Joback Method
cpg	1321.00	J/mol×K	1021.92	Joback Method
cpg	1337.36	J/mol×K	1059.24	Joback Method
cpg	1351.96	J/mol×K	1096.56	Joback Method
cpg	1364.90	J/mol×K	1133.88	Joback Method
cpg	1376.25	J/mol×K	1171.20	Joback Method
dvisc	0.0005875	Pa×s	526.95	Joback Method

dvisc	0.0002615	Pa×s	597.00	Joback Method
dvisc	0.0001380	Pa×s	667.06	Joback Method
dvisc	0.0000822	Pa×s	737.12	Joback Method
dvisc	0.0000536	Pa×s	807.17	Joback Method
dvisc	0.0000374	Pa×s	877.23	Joback Method
dvisc	0.0000275	Pa×s	947.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393396&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