Glutaric acid, 3-methylbut-2-en cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H34O4/c1-15(2)13-14-23-18(21)7-6-8-19(22)24-17-11-9-16(10-12-17)20(3

InchiKey: SZOPDQQSOAVDTG-UHFFFAOYSA-N

Formula: C20H34O4

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

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-259.07	kJ/mol	Joback Method
hf	-813.07	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	77.29	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.814		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	825.27	K	Joback Method
tc	1032.08	K	Joback Method
tf	446.00	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.37	J/mol×K	825.27	Joback Method
cpg	963.62	J/mol×K	859.74	Joback Method
cpg	981.51	J/mol×K	894.21	Joback Method
cpg	998.11	J/mol×K	928.67	Joback Method
cpg	1013.45	J/mol×K	963.14	Joback Method
cpg	1027.60	J/mol×K	997.61	Joback Method
cpg	1040.59	J/mol×K	1032.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393387&Units=SI

Legend

cpg:	Ideal gas heat capacity
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