Glutaric acid, but-3-yn-2-yl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C19H30O4/c1-6-14(2)22-17(20)8-7-9-18(21)23-16-12-10-15(11-13-16)19(3,4)5

InchiKey: WIVCEQKUHPDBPG-UHFFFAOYSA-N

Formula: C19H30O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OC1CCC(C(C)(C)C)CC1

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-118.53	kJ/mol	Joback Method
hf	-613.24	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.870		Crippen Method
mcvol	273.990	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2091.00		NIST Webbook
tb	788.03	K	Joback Method
tc	999.13	K	Joback Method
tf	485.74	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.62	J/mol×K	788.03	Joback Method
cpg	874.71	J/mol×K	823.21	Joback Method
cpg	892.42	J/mol×K	858.40	Joback Method
cpg	908.80	J/mol×K	893.58	Joback Method
cpg	923.89	J/mol×K	928.76	Joback Method
cpg	937.73	J/mol×K	963.95	Joback Method
cpg	950.36	J/mol×K	999.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393384&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

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