Glutaric acid, 1,1,1-trifluoroprop-2-yl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C18H29F3O4/c1-12(18(19,20)21)24-15(22)6-5-7-16(23)25-14-10-8-13(9-11-14

InchiKey: PFBHVRMGFSSGLT-UHFFFAOYSA-N

Formula: C18H29F3O4

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

Mol. weight [g/mol]: 366.42

Physical Properties

Property code	Value	Unit	Source
gf	-931.61	kJ/mol	Joback Method
hf	-1481.58	kJ/mol	Joback Method
hfus	31.75	kJ/mol	Joback Method
hvap	68.66	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.799		Crippen Method
mcvol	273.810	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
tb	769.61	K	Joback Method
tc	962.85	K	Joback Method
tf	431.69	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.74	J/mol×K	769.61	Joback Method
cpg	892.95	J/mol×K	801.82	Joback Method
cpg	909.92	J/mol×K	834.02	Joback Method
cpg	925.70	J/mol×K	866.23	Joback Method
cpg	940.33	J/mol×K	898.44	Joback Method
cpg	953.85	J/mol×K	930.64	Joback Method
cpg	966.31	J/mol×K	962.85	Joback Method

Sources

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=U393397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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