Glutaric acid, 2,2,3,3-tetrafluoropropyl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C18H28F4O4/c1-17(2,3)12-7-9-13(10-8-12)26-15(24)6-4-5-14(23)25-11-18(21
InchiKey: CJYVEPOSAOZKAN-UHFFFAOYSA-N
Formula: C18H28F4O4
SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)CC1
Mol. weight [g/mol]: 384.41

Physical Properties

Property code	Value	Unit	Source
gf	-1126.42	kJ/mol	Joback Method
hf	-1677.69	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	67.85	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.748		Crippen Method
mcvol	275.580	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		NIST Webbook
tb	768.88	K	Joback Method
tc	957.20	K	Joback Method
tf	432.28	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.31	J/mol×K	768.88	Joback Method
cpg	899.99	J/mol×K	800.27	Joback Method
cpg	916.48	J/mol×K	831.65	Joback Method
cpg	931.83	J/mol×K	863.04	Joback Method
cpg	946.08	J/mol×K	894.43	Joback Method
cpg	959.28	J/mol×K	925.82	Joback Method
cpg	971.45	J/mol×K	957.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393382&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
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