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

Inchi: InChI=1S/C17H27F3O4/c1-11(17(18,19)20)23-14(21)9-10-15(22)24-13-7-5-12(6-8-13)16

InchiKey: JTHYTTQHTREKJC-UHFFFAOYSA-N

Formula: C17H27F3O4

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

Mol. weight [g/mol]: 352.39

Physical Properties

Property code	Value	Unit	Source
gf	-940.03	kJ/mol	Joback Method
hf	-1460.94	kJ/mol	Joback Method
hfus	29.16	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.409		Crippen Method
mcvol	259.720	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
tb	746.73	K	Joback Method
tc	940.53	K	Joback Method
tf	420.42	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.38	J/mol×K	746.73	Joback Method
cpg	834.49	J/mol×K	779.03	Joback Method
cpg	851.38	J/mol×K	811.33	Joback Method
cpg	867.09	J/mol×K	843.63	Joback Method
cpg	881.66	J/mol×K	875.93	Joback Method
cpg	895.14	J/mol×K	908.23	Joback Method
cpg	907.57	J/mol×K	940.53	Joback Method

Sources

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=U390193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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