Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C19H26F8O4/c1-16(2,3)11-4-6-12(7-5-11)31-14(29)9-8-13(28)30-10-17(22,23)

InchiKey: ALFDCIGAPMNZBT-UHFFFAOYSA-N

Formula: C19H26F8O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC1

Mol. weight [g/mol]: 470.39

Physical Properties

Property code	Value	Unit	Source
gf	-1891.56	kJ/mol	Joback Method
hf	-2500.27	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.629		Crippen Method
mcvol	296.750	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook
tb	782.38	K	Joback Method
tc	964.95	K	Joback Method
tf	450.75	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.19	J/mol×K	782.38	Joback Method
cpg	990.67	J/mol×K	812.81	Joback Method
cpg	1005.99	J/mol×K	843.24	Joback Method
cpg	1020.24	J/mol×K	873.66	Joback Method
cpg	1033.47	J/mol×K	904.09	Joback Method
cpg	1045.76	J/mol×K	934.52	Joback Method
cpg	1057.16	J/mol×K	964.95	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=U390195&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