Succinic acid, 2-methylhex-3-yl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C19H25F3O4/c1-4-8-15(13(2)3)25-16(23)11-12-17(24)26-18(19(20,21)22)14-9

InchiKey: PXGXUFPLTBGUQJ-UHFFFAOYSA-N

Formula: C19H25F3O4

SMILES: CCCC(OC(=O)CCC(=O)OC(c1ccccc1)C(F)(F)F)C(C)C

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-835.24	kJ/mol	Joback Method
hf	-1301.48	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.981		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	806.64	K	Joback Method
tc	1002.54	K	Joback Method
tf	433.82	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.14	J/mol×K	806.64	Joback Method
cpg	860.38	J/mol×K	839.29	Joback Method
cpg	874.53	J/mol×K	871.94	Joback Method
cpg	887.64	J/mol×K	904.59	Joback Method
cpg	899.75	J/mol×K	937.24	Joback Method
cpg	910.90	J/mol×K	969.89	Joback Method
cpg	921.13	J/mol×K	1002.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381572&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