Succinic acid, 2-methylhex-3-yl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C19H23F5O4/c1-5-6-11(9(2)3)28-13(26)8-7-12(25)27-10(4)14-15(20)17(22)19

InchiKey: CBQNEOVMLLYTJW-UHFFFAOYSA-N

Formula: C19H23F5O4

SMILES: CCCC(OC(=O)CCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 410.38

Physical Properties

Property code	Value	Unit	Source
gf	-1275.85	kJ/mol	Joback Method
hf	-1742.30	kJ/mol	Joback Method
hfus	47.47	kJ/mol	Joback Method
hvap	76.54	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.134		Crippen Method
mcvol	278.540	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	1956.00		NIST Webbook
rinpol	1956.00		NIST Webbook
tb	833.31	K	Joback Method
tc	1023.39	K	Joback Method
tf	495.18	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.88	J/mol×K	833.31	Joback Method
cpg	868.98	J/mol×K	864.99	Joback Method
cpg	882.07	J/mol×K	896.67	Joback Method
cpg	894.16	J/mol×K	928.35	Joback Method
cpg	905.25	J/mol×K	960.03	Joback Method
cpg	915.35	J/mol×K	991.71	Joback Method
cpg	924.46	J/mol×K	1023.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380825&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

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