Succinic acid, 2-fluorophenethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H27FO4/c1-4-7-17(14(2)3)24-19(22)11-10-18(21)23-13-12-15-8-5-6-9-16(1

InchiKey: QPKCNZBYHMFZTF-UHFFFAOYSA-N

Formula: C19H27FO4

SMILES: CCCC(OC(=O)CCC(=O)OCCc1ccccc1F)C(C)C

Mol. weight [g/mol]: 338.41

Physical Properties

Property code	Value	Unit	Source
gf	-455.65	kJ/mol	Joback Method
hf	-906.70	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	77.55	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.059		Crippen Method
mcvol	271.460	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2194.00		NIST Webbook
tb	816.75	K	Joback Method
tc	1015.50	K	Joback Method
tf	457.74	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.58	J/mol×K	816.75	Joback Method
cpg	843.32	J/mol×K	849.87	Joback Method
cpg	857.97	J/mol×K	883.00	Joback Method
cpg	871.53	J/mol×K	916.12	Joback Method
cpg	884.03	J/mol×K	949.25	Joback Method
cpg	895.49	J/mol×K	982.37	Joback Method
cpg	905.94	J/mol×K	1015.50	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=U381403&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