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

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

InchiKey: SYSOZAOBFYGBSY-UHFFFAOYSA-N

Formula: C19H27FO4

SMILES: CCCC(OC(=O)CCC(=O)OC(C)c1ccccc1F)C(C)C

Mol. weight [g/mol]: 338.41

Physical Properties

Property code	Value	Unit	Source
gf	-458.09	kJ/mol	Joback Method
hf	-911.98	kJ/mol	Joback Method
hfus	36.70	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.578		Crippen Method
mcvol	271.460	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	816.31	K	Joback Method
tc	1017.09	K	Joback Method
tf	442.74	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.11	J/mol×K	816.31	Joback Method
cpg	844.01	J/mol×K	849.77	Joback Method
cpg	858.77	J/mol×K	883.24	Joback Method
cpg	872.43	J/mol×K	916.70	Joback Method
cpg	884.99	J/mol×K	950.16	Joback Method
cpg	896.48	J/mol×K	983.62	Joback Method
cpg	906.91	J/mol×K	1017.09	Joback Method

Sources

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=U381394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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