Succinic acid, 1-(2,6-difluorophenyl)ethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H26F2O4/c1-5-7-16(12(2)3)25-18(23)11-10-17(22)24-13(4)19-14(20)8-6-9

InchiKey: NLOFJSOJTRXXOT-UHFFFAOYSA-N

Formula: C19H26F2O4

SMILES: CCCC(OC(=O)CCC(=O)OC(C)c1c(F)cccc1F)C(C)C

Mol. weight [g/mol]: 356.40

Physical Properties

Property code	Value	Unit	Source
gf	-662.53	kJ/mol	Joback Method
hf	-1119.56	kJ/mol	Joback Method
hfus	39.39	kJ/mol	Joback Method
hvap	77.00	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.717		Crippen Method
mcvol	273.230	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tb	820.56	K	Joback Method
tc	1017.56	K	Joback Method
tf	455.85	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.88	J/mol×K	820.56	Joback Method
cpg	850.23	J/mol×K	853.39	Joback Method
cpg	864.50	J/mol×K	886.23	Joback Method
cpg	877.69	J/mol×K	919.06	Joback Method
cpg	889.83	J/mol×K	951.89	Joback Method
cpg	900.93	J/mol×K	984.72	Joback Method
cpg	911.00	J/mol×K	1017.56	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=U381421&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