Succinic acid, 2-fluorophenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C17H23FO4/c1-11(2)17(12(3)4)22-16(20)10-9-15(19)21-14-8-6-5-7-13(14)18/h

InchiKey: PRRGJKHCVOAJGJ-UHFFFAOYSA-N

Formula: C17H23FO4

SMILES: CC(C)C(OC(=O)CCC(=O)Oc1ccccc1F)C(C)C

Mol. weight [g/mol]: 310.36

Physical Properties

Property code	Value	Unit	Source
gf	-474.93	kJ/mol	Joback Method
hf	-870.70	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.735		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	770.55	K	Joback Method
tc	972.72	K	Joback Method
tf	420.20	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.62	J/mol×K	770.55	Joback Method
cpg	729.10	J/mol×K	804.25	Joback Method
cpg	743.52	J/mol×K	837.94	Joback Method
cpg	756.89	J/mol×K	871.64	Joback Method
cpg	769.23	J/mol×K	905.33	Joback Method
cpg	780.56	J/mol×K	939.03	Joback Method
cpg	790.89	J/mol×K	972.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390506&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