Succinic acid, 2-isopropoxyphenyl 3-fluorophenyl ester

Inchi: InChI=1S/C19H19FO5/c1-13(2)23-16-8-3-4-9-17(16)25-19(22)11-10-18(21)24-15-7-5-6-1

InchiKey: XKURYMYMMQLGFH-UHFFFAOYSA-N

Formula: C19H19FO5

SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 346.35

Physical Properties

Property code	Value	Unit	Source
gf	-455.43	kJ/mol	Joback Method
hf	-808.58	kJ/mol	Joback Method
hfus	38.59	kJ/mol	Joback Method
hvap	83.28	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.904		Crippen Method
mcvol	253.570	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	2454.00		NIST Webbook
tb	871.27	K	Joback Method
tc	1092.83	K	Joback Method
tf	533.91	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.06	J/mol×K	871.27	Joback Method
cpg	771.02	J/mol×K	908.20	Joback Method
cpg	782.67	J/mol×K	945.12	Joback Method
cpg	793.01	J/mol×K	982.05	Joback Method
cpg	802.06	J/mol×K	1018.97	Joback Method
cpg	809.84	J/mol×K	1055.90	Joback Method
cpg	816.35	J/mol×K	1092.83	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=U357971&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