Succinic acid, 2-fluorophenyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C16H21FO4/c1-11(16(2,3)4)20-14(18)9-10-15(19)21-13-8-6-5-7-12(13)17/h5-8

InchiKey: MLIYEOSHGIKZQU-UHFFFAOYSA-N

Formula: C16H21FO4

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

Mol. weight [g/mol]: 296.33

Physical Properties

Property code	Value	Unit	Source
gf	-475.63	kJ/mol	Joback Method
hf	-848.25	kJ/mol	Joback Method
hfus	28.57	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.489		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	745.32	K	Joback Method
tc	951.54	K	Joback Method
tf	441.35	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.88	J/mol×K	745.32	Joback Method
cpg	673.97	J/mol×K	779.69	Joback Method
cpg	688.02	J/mol×K	814.06	Joback Method
cpg	701.06	J/mol×K	848.43	Joback Method
cpg	713.13	J/mol×K	882.80	Joback Method
cpg	724.24	J/mol×K	917.17	Joback Method
cpg	734.44	J/mol×K	951.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390624&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

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