Succinic acid, 2-fluorophenyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C18H17FO4/c1-12-6-5-9-15(13(12)2)22-17(20)10-11-18(21)23-16-8-4-3-7-14(1

InchiKey: IIUMDBXSGZFGPW-UHFFFAOYSA-N

Formula: C18H17FO4

SMILES: Cc1cccc(OC(=O)CCC(=O)Oc2ccccc2F)c1C

Mol. weight [g/mol]: 316.32

Physical Properties

Property code	Value	Unit	Source
gf	-366.04	kJ/mol	Joback Method
hf	-661.91	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.734		Crippen Method
mcvol	233.610	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2411.00		NIST Webbook
rinpol	2411.00		NIST Webbook
tb	831.39	K	Joback Method
tc	1053.79	K	Joback Method
tf	527.93	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.21	J/mol×K	831.39	Joback Method
cpg	686.40	J/mol×K	868.46	Joback Method
cpg	698.42	J/mol×K	905.52	Joback Method
cpg	709.29	J/mol×K	942.59	Joback Method
cpg	719.03	J/mol×K	979.66	Joback Method
cpg	727.66	J/mol×K	1016.73	Joback Method
cpg	735.19	J/mol×K	1053.79	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=U390022&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