Succinic acid, 2-fluorophenyl 3-methoxyphenyl ester

Inchi: InChI=1S/C17H15FO5/c1-21-12-5-4-6-13(11-12)22-16(19)9-10-17(20)23-15-8-3-2-7-14(1

InchiKey: VQWMFRFVLPUNJG-UHFFFAOYSA-N

Formula: C17H15FO5

SMILES: COc1cccc(OC(=O)CCC(=O)Oc2ccccc2F)c1

Mol. weight [g/mol]: 318.30

Physical Properties

Property code	Value	Unit	Source
gf	-469.83	kJ/mol	Joback Method
hf	-762.02	kJ/mol	Joback Method
hfus	36.93	kJ/mol	Joback Method
hvap	79.22	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.125		Crippen Method
mcvol	225.390	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	825.95	K	Joback Method
tc	1048.42	K	Joback Method
tf	526.37	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.29	J/mol×K	825.95	Joback Method
cpg	657.84	J/mol×K	863.03	Joback Method
cpg	669.19	J/mol×K	900.11	Joback Method
cpg	679.35	J/mol×K	937.19	Joback Method
cpg	688.32	J/mol×K	974.26	Joback Method
cpg	696.11	J/mol×K	1011.34	Joback Method
cpg	702.72	J/mol×K	1048.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390982&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