Succinic acid, 2-fluorophenyl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C18H17FO5/c1-12-7-8-15(22-2)16(11-12)24-18(21)10-9-17(20)23-14-6-4-3-5-1

InchiKey: LJJNWHJIKLNTIV-UHFFFAOYSA-N

Formula: C18H17FO5

SMILES: COc1ccc(C)cc1OC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 332.32

Physical Properties

Property code	Value	Unit	Source
gf	-471.04	kJ/mol	Joback Method
hf	-794.13	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	82.11	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.434		Crippen Method
mcvol	239.480	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	2492.00		NIST Webbook
rinpol	2492.00		NIST Webbook
tb	853.81	K	Joback Method
tc	1074.95	K	Joback Method
tf	550.16	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.68	J/mol×K	853.81	Joback Method
cpg	712.29	J/mol×K	890.67	Joback Method
cpg	723.66	J/mol×K	927.52	Joback Method
cpg	733.79	J/mol×K	964.38	Joback Method
cpg	742.68	J/mol×K	1001.24	Joback Method
cpg	750.34	J/mol×K	1038.10	Joback Method
cpg	756.76	J/mol×K	1074.95	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=U390960&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