Succinic acid, di(4-fluoro-2-methoxyphenyl) ester

Inchi: InChI=1S/C18H16F2O6/c1-23-15-9-11(19)3-5-13(15)25-17(21)7-8-18(22)26-14-6-4-12(2

InchiKey: HXBYRPGJZRKFMH-UHFFFAOYSA-N

Formula: C18H16F2O6

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 366.31

Physical Properties

Property code	Value	Unit	Source
gf	-780.48	kJ/mol	Joback Method
hf	-1133.93	kJ/mol	Joback Method
hfus	43.01	kJ/mol	Joback Method
hvap	84.36	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.273		Crippen Method
mcvol	247.120	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
tb	880.48	K	Joback Method
tc	1096.04	K	Joback Method
tf	585.50	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.90	J/mol×K	880.48	Joback Method
cpg	743.33	J/mol×K	916.41	Joback Method
cpg	753.48	J/mol×K	952.33	Joback Method
cpg	762.33	J/mol×K	988.26	Joback Method
cpg	769.85	J/mol×K	1024.19	Joback Method
cpg	776.02	J/mol×K	1060.11	Joback Method
cpg	780.83	J/mol×K	1096.04	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=U390908&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