Succinic acid, dodec-2-en-1-yl 2-fluorophenyl ester

Inchi: InChI=1S/C22H31FO4/c1-2-3-4-5-6-7-8-9-10-13-18-26-21(24)16-17-22(25)27-20-15-12-1

InchiKey: GHGKNKVWHZFUGN-JLHYYAGUSA-N

Formula: C22H31FO4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 378.48

Physical Properties

Property code	Value	Unit	Source
gf	-345.29	kJ/mol	Joback Method
hf	-840.84	kJ/mol	Joback Method
hfus	55.24	kJ/mol	Joback Method
hvap	84.96	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.751		Crippen Method
mcvol	309.430	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	890.43	K	Joback Method
tc	1093.84	K	Joback Method
tf	516.47	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.21	J/mol×K	890.43	Joback Method
cpg	993.01	J/mol×K	924.33	Joback Method
cpg	1007.69	J/mol×K	958.23	Joback Method
cpg	1021.29	J/mol×K	992.14	Joback Method
cpg	1033.84	J/mol×K	1026.04	Joback Method
cpg	1045.40	J/mol×K	1059.94	Joback Method
cpg	1056.00	J/mol×K	1093.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390317&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