Succinic acid, 2-fluorophenyl oct-1-en-3-yl ester

Inchi: InChI=1S/C18H23FO4/c1-3-5-6-9-14(4-2)22-17(20)12-13-18(21)23-16-11-8-7-10-15(16)1

InchiKey: NMCVKQSXAYZNJX-UHFFFAOYSA-N

Formula: C18H23FO4

SMILES: C=CC(CCCCC)OC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 322.37

Physical Properties

Property code	Value	Unit	Source
gf	-373.79	kJ/mol	Joback Method
hf	-755.35	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.189		Crippen Method
mcvol	253.070	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	790.99	K	Joback Method
tc	989.60	K	Joback Method
tf	459.71	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.18	J/mol×K	790.99	Joback Method
cpg	758.02	J/mol×K	824.09	Joback Method
cpg	771.86	J/mol×K	857.19	Joback Method
cpg	784.71	J/mol×K	890.29	Joback Method
cpg	796.60	J/mol×K	923.40	Joback Method
cpg	807.55	J/mol×K	956.50	Joback Method
cpg	817.57	J/mol×K	989.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391321&Units=SI

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