Succinic acid, 2-fluorophenyl hex-5-en-1-yl ester

Inchi: InChI=1S/C16H19FO4/c1-2-3-4-7-12-20-15(18)10-11-16(19)21-14-9-6-5-8-13(14)17/h2,5

InchiKey: XDQGNEFVRLPKDZ-UHFFFAOYSA-N

Formula: C16H19FO4

SMILES: C=CCCCCOC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 294.32

Physical Properties

Property code	Value	Unit	Source
gf	-388.19	kJ/mol	Joback Method
hf	-708.79	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	70.97	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.411		Crippen Method
mcvol	224.890	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	745.67	K	Joback Method
tc	943.52	K	Joback Method
tf	452.17	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.21	J/mol×K	745.67	Joback Method
cpg	645.23	J/mol×K	778.65	Joback Method
cpg	658.36	J/mol×K	811.62	Joback Method
cpg	670.60	J/mol×K	844.60	Joback Method
cpg	681.96	J/mol×K	877.57	Joback Method
cpg	692.47	J/mol×K	910.55	Joback Method
cpg	702.15	J/mol×K	943.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391283&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

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