Succinic acid, 2-fluorophenyl cis-hex-2-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/h4-9

InchiKey: RFJSSZVQOLUYHN-DAXSKMNVSA-N

Formula: C16H19FO4

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

Mol. weight [g/mol]: 294.32

Physical Properties

Property code	Value	Unit	Source
gf	-395.81	kJ/mol	Joback Method
hf	-717.00	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.411		Crippen Method
mcvol	224.890	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
tb	753.15	K	Joback Method
tc	954.26	K	Joback Method
tf	448.85	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.69	J/mol×K	753.15	Joback Method
cpg	645.72	J/mol×K	786.67	Joback Method
cpg	658.84	J/mol×K	820.19	Joback Method
cpg	671.08	J/mol×K	853.71	Joback Method
cpg	682.46	J/mol×K	887.22	Joback Method
cpg	693.00	J/mol×K	920.74	Joback Method
cpg	702.73	J/mol×K	954.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391301&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