Succinic acid, 2-fluorophenyl pent-4-en-1-yl ester

Inchi: InChI=1S/C15H17FO4/c1-2-3-6-11-19-14(17)9-10-15(18)20-13-8-5-4-7-12(13)16/h2,4-5,

InchiKey: LHVZFKCEINVLGF-UHFFFAOYSA-N

Formula: C15H17FO4

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

Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-396.61	kJ/mol	Joback Method
hf	-688.15	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.021		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	722.79	K	Joback Method
tc	922.17	K	Joback Method
tf	440.90	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.11	J/mol×K	722.79	Joback Method
cpg	590.75	J/mol×K	756.02	Joback Method
cpg	603.52	J/mol×K	789.25	Joback Method
cpg	615.44	J/mol×K	822.48	Joback Method
cpg	626.52	J/mol×K	855.71	Joback Method
cpg	636.77	J/mol×K	888.94	Joback Method
cpg	646.21	J/mol×K	922.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391067&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