Succinic acid, 2-fluorophenyl cis-pent-2-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/h3-8H,2

InchiKey: IPBHQNVRPWIWJG-UTCJRWHESA-N

Formula: C15H17FO4

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

Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-404.23	kJ/mol	Joback Method
hf	-696.36	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	69.38	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.021		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	730.27	K	Joback Method
tc	933.11	K	Joback Method
tf	437.58	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.49	J/mol×K	730.27	Joback Method
cpg	591.14	J/mol×K	764.08	Joback Method
cpg	603.91	J/mol×K	797.88	Joback Method
cpg	615.82	J/mol×K	831.69	Joback Method
cpg	626.90	J/mol×K	865.50	Joback Method
cpg	637.17	J/mol×K	899.30	Joback Method
cpg	646.64	J/mol×K	933.11	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=U391261&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