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

Inchi: InChI=1S/C14H15FO4/c1-2-3-10-18-13(16)8-9-14(17)19-12-7-5-4-6-11(12)15/h2,4-7H,1,

InchiKey: OIMODGFVSHZNKI-UHFFFAOYSA-N

Formula: C14H15FO4

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

Mol. weight [g/mol]: 266.26

Physical Properties

Property code	Value	Unit	Source
gf	-405.03	kJ/mol	Joback Method
hf	-667.51	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.631		Crippen Method
mcvol	196.710	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1838.00		NIST Webbook
rinpol	1838.00		NIST Webbook
tb	699.91	K	Joback Method
tc	901.29	K	Joback Method
tf	429.63	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.19	J/mol×K	699.91	Joback Method
cpg	537.39	J/mol×K	733.47	Joback Method
cpg	549.75	J/mol×K	767.04	Joback Method
cpg	561.30	J/mol×K	800.60	Joback Method
cpg	572.04	J/mol×K	834.16	Joback Method
cpg	581.98	J/mol×K	867.73	Joback Method
cpg	591.14	J/mol×K	901.29	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=U391193&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