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

Inchi: InChI=1S/C15H17FO4/c1-11(2)9-10-19-14(17)7-8-15(18)20-13-6-4-3-5-12(13)16/h3-6H,1

InchiKey: FFYXXGKSIWYPPG-UHFFFAOYSA-N

Formula: C15H17FO4

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

Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-405.16	kJ/mol	Joback Method
hf	-697.94	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	68.83	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.021		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	722.67	K	Joback Method
tc	924.63	K	Joback Method
tf	426.94	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.78	J/mol×K	722.67	Joback Method
cpg	590.58	J/mol×K	756.33	Joback Method
cpg	603.49	J/mol×K	789.99	Joback Method
cpg	615.53	J/mol×K	823.65	Joback Method
cpg	626.71	J/mol×K	857.31	Joback Method
cpg	637.06	J/mol×K	890.97	Joback Method
cpg	646.57	J/mol×K	924.63	Joback Method

Sources

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=U391136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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