Succinic acid, 2-fluorophenyl 2-methoxyethyl ester

Inchi: InChI=1S/C13H15FO5/c1-17-8-9-18-12(15)6-7-13(16)19-11-5-3-2-4-10(11)14/h2-5H,6-9

InchiKey: GISZEGIAWRWBAZ-UHFFFAOYSA-N

Formula: C13H15FO5

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

Mol. weight [g/mol]: 270.25

Physical Properties

Property code	Value	Unit	Source
gf	-606.29	kJ/mol	Joback Method
hf	-904.52	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.701		Crippen Method
mcvol	192.790	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	702.77	K	Joback Method
tc	901.90	K	Joback Method
tf	442.35	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.45	J/mol×K	702.77	Joback Method
cpg	534.50	J/mol×K	735.96	Joback Method
cpg	546.75	J/mol×K	769.15	Joback Method
cpg	558.19	J/mol×K	802.34	Joback Method
cpg	568.80	J/mol×K	835.52	Joback Method
cpg	578.59	J/mol×K	868.71	Joback Method
cpg	587.54	J/mol×K	901.90	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=U390740&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