Succinic acid, 1,1,1-trifluoroprop-2-yl 2-fluorophenyl ester

Inchi: InChI=1S/C13H12F4O4/c1-8(13(15,16)17)20-11(18)6-7-12(19)21-10-5-3-2-4-9(10)14/h2-

InchiKey: FNXINDDRJOLCEU-UHFFFAOYSA-N

Formula: C13H12F4O4

SMILES: CC(OC(=O)CCC(=O)Oc1ccccc1F)C(F)(F)F

Mol. weight [g/mol]: 308.23

Physical Properties

Property code	Value	Unit	Source
gf	-1085.32	kJ/mol	Joback Method
hf	-1374.66	kJ/mol	Joback Method
hfus	30.04	kJ/mol	Joback Method
hvap	60.83	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.005		Crippen Method
mcvol	192.230	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	674.49	K	Joback Method
tc	864.84	K	Joback Method
tf	409.31	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.03	J/mol×K	674.49	Joback Method
cpg	535.29	J/mol×K	706.21	Joback Method
cpg	546.75	J/mol×K	737.94	Joback Method
cpg	557.44	J/mol×K	769.66	Joback Method
cpg	567.37	J/mol×K	801.39	Joback Method
cpg	576.58	J/mol×K	833.11	Joback Method
cpg	585.07	J/mol×K	864.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390301&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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