Succinic acid, 2-ethylhexyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C18H23F3O4/c1-3-5-6-12(4-2)11-24-15(22)9-10-16(23)25-14-8-7-13(19)17(20

InchiKey: JGVDMSCSGKTHPK-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-870.51	kJ/mol	Joback Method
hf	-1295.94	kJ/mol	Joback Method
hfus	46.54	kJ/mol	Joback Method
hvap	75.40	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.549		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	802.81	K	Joback Method
tc	992.51	K	Joback Method
tf	487.69	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.91	J/mol×K	802.81	Joback Method
cpg	797.25	J/mol×K	834.43	Joback Method
cpg	810.64	J/mol×K	866.04	Joback Method
cpg	823.10	J/mol×K	897.66	Joback Method
cpg	834.63	J/mol×K	929.28	Joback Method
cpg	845.24	J/mol×K	960.89	Joback Method
cpg	854.94	J/mol×K	992.51	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=U390763&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