Succinic acid, 2-methylpent-3-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H19F3O4/c1-4-11(9(2)3)22-13(20)7-8-14(21)23-12-6-5-10(17)15(18)16(12

InchiKey: QOASOAGGAWRJMJ-UHFFFAOYSA-N

Formula: C16H19F3O4

SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-889.79	kJ/mol	Joback Method
hf	-1259.94	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.767		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	756.61	K	Joback Method
tc	947.19	K	Joback Method
tf	450.15	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.03	J/mol×K	756.61	Joback Method
cpg	684.79	J/mol×K	788.37	Joback Method
cpg	697.68	J/mol×K	820.14	Joback Method
cpg	709.70	J/mol×K	851.90	Joback Method
cpg	720.87	J/mol×K	883.66	Joback Method
cpg	731.17	J/mol×K	915.42	Joback Method
cpg	740.63	J/mol×K	947.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390757&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