Succinic acid, dodec-2-en-1-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C22H29F3O4/c1-2-3-4-5-6-7-8-9-10-11-16-28-19(26)14-15-20(27)29-18-13-12

InchiKey: RIUDNWPCYWCJBJ-ZHACJKMWSA-N

Formula: C22H29F3O4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 414.46

Physical Properties

Property code	Value	Unit	Source
gf	-754.17	kJ/mol	Joback Method
hf	-1256.00	kJ/mol	Joback Method
hfus	60.63	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	6.030		Crippen Method
mcvol	312.970	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	2603.00		NIST Webbook
rinpol	2603.00		NIST Webbook
tb	898.93	K	Joback Method
tc	1100.99	K	Joback Method
tf	542.69	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.10	J/mol×K	898.93	Joback Method
cpg	1005.28	J/mol×K	932.61	Joback Method
cpg	1019.35	J/mol×K	966.28	Joback Method
cpg	1032.34	J/mol×K	999.96	Joback Method
cpg	1044.27	J/mol×K	1033.64	Joback Method
cpg	1055.19	J/mol×K	1067.31	Joback Method
cpg	1065.12	J/mol×K	1100.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390772&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

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