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

Inchi: InChI=1S/C20H27F3O4/c1-3-4-5-6-7-8-9-14(2)26-17(24)12-13-18(25)27-16-11-10-15(21
InchiKey: XXUFLKYTCWDPQW-UHFFFAOYSA-N
Formula: C20H27F3O4
SMILES: CCCCCCCCC(C)OC(=O)CCC(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-853.67	kJ/mol	Joback Method
hf	-1337.22	kJ/mol	Joback Method
hfus	51.72	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.472		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tb	848.57	K	Joback Method
tc	1042.25	K	Joback Method
tf	510.23	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.97	J/mol×K	848.57	Joback Method
cpg	913.99	J/mol×K	880.85	Joback Method
cpg	927.94	J/mol×K	913.13	Joback Method
cpg	940.84	J/mol×K	945.41	Joback Method
cpg	952.69	J/mol×K	977.69	Joback Method
cpg	963.52	J/mol×K	1009.97	Joback Method
cpg	973.34	J/mol×K	1042.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390767&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