Succinic acid, dec-2-yl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C21H28F4O4/c1-3-4-5-6-7-8-10-15(2)28-18(26)13-14-19(27)29-17-12-9-11-16

InchiKey: DYIKHQMVIONQHS-UHFFFAOYSA-N

Formula: C21H28F4O4

SMILES: CCCCCCCCC(C)OC(=O)CCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 420.44

Physical Properties

Property code	Value	Unit	Source
gf	-1027.59	kJ/mol	Joback Method
hf	-1551.25	kJ/mol	Joback Method
hfus	50.37	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.212		Crippen Method
mcvol	304.950	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	862.51	K	Joback Method
tc	1057.99	K	Joback Method
tf	511.99	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.93	J/mol×K	862.51	Joback Method
cpg	982.03	J/mol×K	895.09	Joback Method
cpg	996.04	J/mol×K	927.67	Joback Method
cpg	1009.01	J/mol×K	960.25	Joback Method
cpg	1020.96	J/mol×K	992.83	Joback Method
cpg	1031.94	J/mol×K	1025.41	Joback Method
cpg	1041.98	J/mol×K	1057.99	Joback Method

Sources

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=U390789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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