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

Inchi: InChI=1S/C18H22F4O4/c1-3-4-5-7-12(2)25-15(23)10-11-16(24)26-14-9-6-8-13(17(14)19

InchiKey: VQYJDLMKAUOQFP-UHFFFAOYSA-N

Formula: C18H22F4O4

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

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1052.85	kJ/mol	Joback Method
hf	-1489.33	kJ/mol	Joback Method
hfus	42.60	kJ/mol	Joback Method
hvap	72.62	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.042		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1365.67	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	793.87	K	Joback Method
tc	983.08	K	Joback Method
tf	478.18	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.85	J/mol×K	793.87	Joback Method
cpg	806.95	J/mol×K	825.41	Joback Method
cpg	820.11	J/mol×K	856.94	Joback Method
cpg	832.35	J/mol×K	888.48	Joback Method
cpg	843.70	J/mol×K	920.01	Joback Method
cpg	854.19	J/mol×K	951.55	Joback Method
cpg	863.84	J/mol×K	983.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390783&Units=SI

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