Succinic acid, 2-fluoro-6-(trifluoromethyl)benzyl pentadecyl ester

Inchi: InChI=1S/C27H40F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-34-25(32)18-19-26(33)35
InchiKey: SWTYRDLTXYWRSI-UHFFFAOYSA-N
Formula: C27H40F4O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 504.60

Physical Properties

Property code	Value	Unit	Source
gf	-974.63	kJ/mol	Joback Method
hf	-1669.81	kJ/mol	Joback Method
hfus	69.43	kJ/mol	Joback Method
hvap	93.04	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	8.302		Crippen Method
mcvol	389.490	ml/mol	McGowan Method
pc	781.12	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	1000.23	K	Joback Method
tc	1234.50	K	Joback Method
tf	594.61	K	Joback Method
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.58	J/mol×K	1000.23	Joback Method
cpg	1350.41	J/mol×K	1039.28	Joback Method
cpg	1366.62	J/mol×K	1078.32	Joback Method
cpg	1381.29	J/mol×K	1117.37	Joback Method
cpg	1394.51	J/mol×K	1156.41	Joback Method
cpg	1406.38	J/mol×K	1195.46	Joback Method
cpg	1416.99	J/mol×K	1234.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381645&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