Sebacic acid, 3,5-difluorophenyl undecyl ester

Inchi: InChI=1S/C27H42F2O4/c1-2-3-4-5-6-7-10-13-16-19-32-26(30)17-14-11-8-9-12-15-18-27
InchiKey: JCRWRTJCORKIAL-UHFFFAOYSA-N
Formula: C27H42F2O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-587.85	kJ/mol	Joback Method
hf	-1268.84	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	95.97	kJ/mol	Joback Method
log10ws	-9.26		Crippen Method
logp	8.065		Crippen Method
mcvol	385.950	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	3163.00		NIST Webbook
tb	1004.92	K	Joback Method
tc	1237.97	K	Joback Method
tf	591.01	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.25	J/mol×K	1004.92	Joback Method
cpg	1337.11	J/mol×K	1043.76	Joback Method
cpg	1353.20	J/mol×K	1082.60	Joback Method
cpg	1367.59	J/mol×K	1121.44	Joback Method
cpg	1380.33	J/mol×K	1160.28	Joback Method
cpg	1391.48	J/mol×K	1199.12	Joback Method
cpg	1401.11	J/mol×K	1237.97	Joback Method

Sources

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=U354533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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