Sebacic acid, 3,5-difluorophenyl tetradecyl ester

Inchi: InChI=1S/C30H48F2O4/c1-2-3-4-5-6-7-8-9-10-13-16-19-22-35-29(33)20-17-14-11-12-15

InchiKey: KOWFMXBIUZDZAK-UHFFFAOYSA-N

Formula: C30H48F2O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 510.70

Physical Properties

Property code	Value	Unit	Source
gf	-562.59	kJ/mol	Joback Method
hf	-1330.76	kJ/mol	Joback Method
hfus	78.45	kJ/mol	Joback Method
hvap	102.65	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.235		Crippen Method
mcvol	428.220	ml/mol	McGowan Method
pc	694.35	kPa	Joback Method
rinpol	3470.00		NIST Webbook
rinpol	3470.00		NIST Webbook
tb	1073.56	K	Joback Method
tc	1341.16	K	Joback Method
tf	624.82	K	Joback Method
vc	1.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.93	J/mol×K	1073.56	Joback Method
cpg	1528.25	J/mol×K	1118.16	Joback Method
cpg	1545.22	J/mol×K	1162.76	Joback Method
cpg	1559.95	J/mol×K	1207.36	Joback Method
cpg	1572.55	J/mol×K	1251.96	Joback Method
cpg	1583.12	J/mol×K	1296.56	Joback Method
cpg	1591.78	J/mol×K	1341.16	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=U354536&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