Sebacic acid, 3,5-difluorophenyl pentadecyl ester

Inchi: InChI=1S/C31H50F2O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-20-23-36-30(34)21-18-15-12-13

InchiKey: CZGGPLFPONZPLN-UHFFFAOYSA-N

Formula: C31H50F2O4

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

Mol. weight [g/mol]: 524.72

Physical Properties

Property code	Value	Unit	Source
gf	-554.17	kJ/mol	Joback Method
hf	-1351.40	kJ/mol	Joback Method
hfus	81.04	kJ/mol	Joback Method
hvap	104.88	kJ/mol	Joback Method
log10ws	-10.94		Crippen Method
logp	9.625		Crippen Method
mcvol	442.310	ml/mol	McGowan Method
pc	660.51	kPa	Joback Method
rinpol	3588.00		NIST Webbook
tb	1096.44	K	Joback Method
tc	1378.67	K	Joback Method
tf	636.09	K	Joback Method
vc	1.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.68	J/mol×K	1096.44	Joback Method
cpg	1592.55	J/mol×K	1143.48	Joback Method
cpg	1609.81	J/mol×K	1190.52	Joback Method
cpg	1624.61	J/mol×K	1237.56	Joback Method
cpg	1637.06	J/mol×K	1284.60	Joback Method
cpg	1647.32	J/mol×K	1331.64	Joback Method
cpg	1655.51	J/mol×K	1378.67	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=U354537&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