Sebacic acid, 2-fluorophenyl undecyl ester

Inchi: InChI=1S/C27H43FO4/c1-2-3-4-5-6-7-10-13-18-23-31-26(29)21-14-11-8-9-12-15-22-27(3
InchiKey: ZGBLRTJUPXCEBS-UHFFFAOYSA-N
Formula: C27H43FO4
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 450.63

Physical Properties

Property code	Value	Unit	Source
gf	-383.41	kJ/mol	Joback Method
hf	-1061.26	kJ/mol	Joback Method
hfus	67.99	kJ/mol	Joback Method
hvap	96.13	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.926		Crippen Method
mcvol	384.180	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook
tb	1000.67	K	Joback Method
tc	1229.47	K	Joback Method
tf	577.90	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.16	J/mol×K	1000.67	Joback Method
cpg	1331.08	J/mol×K	1038.80	Joback Method
cpg	1347.32	J/mol×K	1076.94	Joback Method
cpg	1361.94	J/mol×K	1115.07	Joback Method
cpg	1375.00	J/mol×K	1153.21	Joback Method
cpg	1386.57	J/mol×K	1191.34	Joback Method
cpg	1396.71	J/mol×K	1229.47	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=U355005&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

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