Succinic acid, 4-fluorophenethyl octadecyl ester

Inchi: InChI=1S/C30H49FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-25-34-29(32)22-23-3

InchiKey: STIXMOJRMBNKPA-UHFFFAOYSA-N

Formula: C30H49FO4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccc(F)cc1

Mol. weight [g/mol]: 492.71

Physical Properties

Property code	Value	Unit	Source
gf	-358.15	kJ/mol	Joback Method
hf	-1123.18	kJ/mol	Joback Method
hfus	75.76	kJ/mol	Joback Method
hvap	102.81	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.496		Crippen Method
mcvol	426.450	ml/mol	McGowan Method
pc	716.83	kPa	Joback Method
rinpol	3291.00		NIST Webbook
rinpol	3291.00		NIST Webbook
tb	1069.31	K	Joback Method
tc	1329.04	K	Joback Method
tf	611.71	K	Joback Method
vc	1.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.27	J/mol×K	1069.31	Joback Method
cpg	1522.55	J/mol×K	1112.60	Joback Method
cpg	1539.65	J/mol×K	1155.89	Joback Method
cpg	1554.68	J/mol×K	1199.17	Joback Method
cpg	1567.76	J/mol×K	1242.46	Joback Method
cpg	1578.99	J/mol×K	1285.75	Joback Method
cpg	1588.48	J/mol×K	1329.04	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=U381310&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