Succinic acid, 4-fluorophenethyl heptadecyl ester

Inchi: InChI=1S/C29H47FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-24-33-28(31)21-22-29(3

InchiKey: JTRWRYSACRLLOE-UHFFFAOYSA-N

Formula: C29H47FO4

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

Mol. weight [g/mol]: 478.68

Physical Properties

Property code	Value	Unit	Source
gf	-366.57	kJ/mol	Joback Method
hf	-1102.54	kJ/mol	Joback Method
hfus	73.17	kJ/mol	Joback Method
hvap	100.58	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.106		Crippen Method
mcvol	412.360	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook
tb	1046.43	K	Joback Method
tc	1294.45	K	Joback Method
tf	600.44	K	Joback Method
vc	1.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.60	J/mol×K	1046.43	Joback Method
cpg	1458.39	J/mol×K	1087.77	Joback Method
cpg	1475.19	J/mol×K	1129.10	Joback Method
cpg	1490.09	J/mol×K	1170.44	Joback Method
cpg	1503.19	J/mol×K	1211.78	Joback Method
cpg	1514.56	J/mol×K	1253.11	Joback Method
cpg	1524.31	J/mol×K	1294.45	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=U381309&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