Succinic acid, 4-fluorophenethyl hexadecyl ester

Inchi: InChI=1S/C28H45FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-23-32-27(30)20-21-28(31)3
InchiKey: JJNLYKGTQJZXJO-UHFFFAOYSA-N
Formula: C28H45FO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccc(F)cc1
Mol. weight [g/mol]: 464.65

Physical Properties

Property code	Value	Unit	Source
gf	-374.99	kJ/mol	Joback Method
hf	-1081.90	kJ/mol	Joback Method
hfus	70.58	kJ/mol	Joback Method
hvap	98.35	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.716		Crippen Method
mcvol	398.270	ml/mol	McGowan Method
pc	796.63	kPa	Joback Method
rinpol	3240.00		NIST Webbook
rinpol	3240.00		NIST Webbook
tb	1023.55	K	Joback Method
tc	1261.30	K	Joback Method
tf	589.17	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1376.21	J/mol×K	1023.55	Joback Method
cpg	1394.55	J/mol×K	1063.17	Joback Method
cpg	1411.06	J/mol×K	1102.80	Joback Method
cpg	1425.83	J/mol×K	1142.42	Joback Method
cpg	1438.92	J/mol×K	1182.05	Joback Method
cpg	1450.41	J/mol×K	1221.67	Joback Method
cpg	1460.37	J/mol×K	1261.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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