Succinic acid, eicosyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C32H49F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-40-25(3

InchiKey: DYZRQOXOKXXGOL-UHFFFAOYSA-N

Formula: C32H49F5O4

SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 592.72

Physical Properties

Property code	Value	Unit	Source
gf	-1161.51	kJ/mol	Joback Method
hf	-2000.06	kJ/mol	Joback Method
hfus	88.18	kJ/mol	Joback Method
hvap	106.25	kJ/mol	Joback Method
log10ws	-12.16		Crippen Method
logp	10.351		Crippen Method
mcvol	461.710	ml/mol	McGowan Method
pc	578.13	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1131.63	K	Joback Method
tc	1464.42	K	Joback Method
tf	671.69	K	Joback Method
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.04	J/mol×K	1131.63	Joback Method
cpg	1672.28	J/mol×K	1187.10	Joback Method
cpg	1688.63	J/mol×K	1242.56	Joback Method
cpg	1701.26	J/mol×K	1298.03	Joback Method
cpg	1710.36	J/mol×K	1353.49	Joback Method
cpg	1716.09	J/mol×K	1408.96	Joback Method
cpg	1718.63	J/mol×K	1464.42	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=U380838&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