Succinic acid, 1-(pentafluorophenyl)ethyl tetradecyl ester

Inchi: InChI=1S/C26H37F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-34-19(32)15-16-20(33)35-1

InchiKey: HMSDMOFAHXXTEM-UHFFFAOYSA-N

Formula: C26H37F5O4

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

Mol. weight [g/mol]: 508.56

Physical Properties

Property code	Value	Unit	Source
gf	-1212.03	kJ/mol	Joback Method
hf	-1876.22	kJ/mol	Joback Method
hfus	72.64	kJ/mol	Joback Method
hvap	92.89	kJ/mol	Joback Method
log10ws	-9.65		Crippen Method
logp	8.011		Crippen Method
mcvol	377.170	ml/mol	McGowan Method
pc	778.94	kPa	Joback Method
rinpol	2788.00		NIST Webbook
tb	994.35	K	Joback Method
tc	1231.40	K	Joback Method
tf	604.07	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.32	J/mol×K	994.35	Joback Method
cpg	1292.50	J/mol×K	1033.86	Joback Method
cpg	1307.80	J/mol×K	1073.37	Joback Method
cpg	1321.24	J/mol×K	1112.88	Joback Method
cpg	1332.86	J/mol×K	1152.38	Joback Method
cpg	1342.71	J/mol×K	1191.89	Joback Method
cpg	1350.81	J/mol×K	1231.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380833&Units=SI

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