Succinic acid, hexadecyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C28H41F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-36-21(34)17-18-22(3

InchiKey: SOUYAIKXGNGDLP-UHFFFAOYSA-N

Formula: C28H41F5O4

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

Mol. weight [g/mol]: 536.61

Physical Properties

Property code	Value	Unit	Source
gf	-1195.19	kJ/mol	Joback Method
hf	-1917.50	kJ/mol	Joback Method
hfus	77.82	kJ/mol	Joback Method
hvap	97.35	kJ/mol	Joback Method
log10ws	-10.49		Crippen Method
logp	8.791		Crippen Method
mcvol	405.350	ml/mol	McGowan Method
pc	701.72	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	1040.11	K	Joback Method
tc	1302.14	K	Joback Method
tf	626.61	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.93	J/mol×K	1040.11	Joback Method
cpg	1418.12	J/mol×K	1083.78	Joback Method
cpg	1433.94	J/mol×K	1127.45	Joback Method
cpg	1447.46	J/mol×K	1171.12	Joback Method
cpg	1458.72	J/mol×K	1214.80	Joback Method
cpg	1467.79	J/mol×K	1258.47	Joback Method
cpg	1474.74	J/mol×K	1302.14	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=U380835&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