Succinic acid, heptadecyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C29H43F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-37-22(35)18-19-2

InchiKey: QOYBSSYEUIGKAN-UHFFFAOYSA-N

Formula: C29H43F5O4

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

Mol. weight [g/mol]: 550.64

Physical Properties

Property code	Value	Unit	Source
gf	-1186.77	kJ/mol	Joback Method
hf	-1938.14	kJ/mol	Joback Method
hfus	80.41	kJ/mol	Joback Method
hvap	99.57	kJ/mol	Joback Method
log10ws	-10.91		Crippen Method
logp	9.181		Crippen Method
mcvol	419.440	ml/mol	McGowan Method
pc	667.35	kPa	Joback Method
rinpol	3046.00		NIST Webbook
rinpol	3046.00		NIST Webbook
tb	1062.99	K	Joback Method
tc	1339.90	K	Joback Method
tf	637.88	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.66	J/mol×K	1062.99	Joback Method
cpg	1481.37	J/mol×K	1109.14	Joback Method
cpg	1497.41	J/mol×K	1155.29	Joback Method
cpg	1510.85	J/mol×K	1201.44	Joback Method
cpg	1521.78	J/mol×K	1247.60	Joback Method
cpg	1530.28	J/mol×K	1293.75	Joback Method
cpg	1536.42	J/mol×K	1339.90	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=U380836&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