Succinic acid, 1-(pentafluorophenyl)ethyl undecyl ester

Inchi: InChI=1S/C23H31F5O4/c1-3-4-5-6-7-8-9-10-11-14-31-16(29)12-13-17(30)32-15(2)18-19

InchiKey: BQIYFYHWPAYYGR-UHFFFAOYSA-N

Formula: C23H31F5O4

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

Mol. weight [g/mol]: 466.48

Physical Properties

Property code	Value	Unit	Source
gf	-1237.29	kJ/mol	Joback Method
hf	-1814.30	kJ/mol	Joback Method
hfus	64.87	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	6.840		Crippen Method
mcvol	334.900	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook
tb	925.71	K	Joback Method
tc	1135.53	K	Joback Method
tf	570.26	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.30	J/mol×K	925.71	Joback Method
cpg	1107.06	J/mol×K	960.68	Joback Method
cpg	1121.43	J/mol×K	995.65	Joback Method
cpg	1134.43	J/mol×K	1030.62	Joback Method
cpg	1146.08	J/mol×K	1065.59	Joback Method
cpg	1156.40	J/mol×K	1100.56	Joback Method
cpg	1165.39	J/mol×K	1135.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380831&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