Succinic acid, 1-(2,6-difluorophenyl)ethyl tridecyl ester

Inchi: InChI=1S/C25H38F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-19-30-23(28)17-18-24(29)31-20(2

InchiKey: DZILCIHWYAGELE-UHFFFAOYSA-N

Formula: C25H38F2O4

SMILES: CCCCCCCCCCCCCOC(=O)CCC(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 440.56

Physical Properties

Property code	Value	Unit	Source
gf	-607.13	kJ/mol	Joback Method
hf	-1232.84	kJ/mol	Joback Method
hfus	61.98	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.203		Crippen Method
mcvol	357.770	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
tb	958.72	K	Joback Method
tc	1174.71	K	Joback Method
tf	553.47	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.93	J/mol×K	958.72	Joback Method
cpg	1211.86	J/mol×K	994.72	Joback Method
cpg	1227.29	J/mol×K	1030.72	Joback Method
cpg	1241.27	J/mol×K	1066.72	Joback Method
cpg	1253.84	J/mol×K	1102.72	Joback Method
cpg	1265.03	J/mol×K	1138.72	Joback Method
cpg	1274.88	J/mol×K	1174.71	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=U381428&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume