Glutaric acid, 1-(2,6-difluorophenyl)ethyl tetradecyl ester

Inchi: InChI=1S/C27H42F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-21-32-25(30)19-16-20-26(31)3

InchiKey: MTLKRPKPEZZKIC-UHFFFAOYSA-N

Formula: C27H42F2O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-590.29	kJ/mol	Joback Method
hf	-1274.12	kJ/mol	Joback Method
hfus	67.16	kJ/mol	Joback Method
hvap	95.59	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	7.984		Crippen Method
mcvol	385.950	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	3102.00		NIST Webbook
rinpol	3102.00		NIST Webbook
tb	1004.48	K	Joback Method
tc	1235.92	K	Joback Method
tf	576.01	K	Joback Method
vc	1.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.57	J/mol×K	1004.48	Joback Method
cpg	1337.24	J/mol×K	1043.05	Joback Method
cpg	1353.17	J/mol×K	1081.63	Joback Method
cpg	1367.39	J/mol×K	1120.20	Joback Method
cpg	1379.97	J/mol×K	1158.78	Joback Method
cpg	1390.97	J/mol×K	1197.35	Joback Method
cpg	1400.44	J/mol×K	1235.92	Joback Method

Sources

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=U377259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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