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

Inchi: InChI=1S/C30H48F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-35-28(33)22-19-2

InchiKey: KEZGDTGVNXDUIG-UHFFFAOYSA-N

Formula: C30H48F2O4

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

Mol. weight [g/mol]: 510.70

Physical Properties

Property code	Value	Unit	Source
gf	-565.03	kJ/mol	Joback Method
hf	-1336.04	kJ/mol	Joback Method
hfus	74.93	kJ/mol	Joback Method
hvap	102.26	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	9.154		Crippen Method
mcvol	428.220	ml/mol	McGowan Method
pc	697.28	kPa	Joback Method
rinpol	3406.00		NIST Webbook
rinpol	3406.00		NIST Webbook
tb	1073.12	K	Joback Method
tc	1337.58	K	Joback Method
tf	609.82	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.09	J/mol×K	1073.12	Joback Method
cpg	1528.10	J/mol×K	1117.20	Joback Method
cpg	1544.79	J/mol×K	1161.27	Joback Method
cpg	1559.27	J/mol×K	1205.35	Joback Method
cpg	1571.63	J/mol×K	1249.43	Joback Method
cpg	1582.00	J/mol×K	1293.50	Joback Method
cpg	1590.47	J/mol×K	1337.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377262&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