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

Inchi: InChI=1S/C29H46F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-34-27(32)21-18-22-2

InchiKey: UUPBAIDEASSMDB-UHFFFAOYSA-N

Formula: C29H46F2O4

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

Mol. weight [g/mol]: 496.67

Physical Properties

Property code	Value	Unit	Source
gf	-573.45	kJ/mol	Joback Method
hf	-1315.40	kJ/mol	Joback Method
hfus	72.34	kJ/mol	Joback Method
hvap	100.04	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	8.764		Crippen Method
mcvol	414.130	ml/mol	McGowan Method
pc	734.03	kPa	Joback Method
rinpol	3306.00		NIST Webbook
tb	1050.24	K	Joback Method
tc	1302.25	K	Joback Method
tf	598.55	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.63	J/mol×K	1050.24	Joback Method
cpg	1464.17	J/mol×K	1092.24	Joback Method
cpg	1480.60	J/mol×K	1134.24	Joback Method
cpg	1495.01	J/mol×K	1176.24	Joback Method
cpg	1507.49	J/mol×K	1218.24	Joback Method
cpg	1518.13	J/mol×K	1260.24	Joback Method
cpg	1527.00	J/mol×K	1302.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377261&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