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

Inchi: InChI=1S/C28H44F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-22-33-26(31)20-17-21-27(3

InchiKey: HJGJDJMBLISUER-UHFFFAOYSA-N

Formula: C28H44F2O4

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

Mol. weight [g/mol]: 482.64

Physical Properties

Property code	Value	Unit	Source
gf	-581.87	kJ/mol	Joback Method
hf	-1294.76	kJ/mol	Joback Method
hfus	69.75	kJ/mol	Joback Method
hvap	97.81	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	8.374		Crippen Method
mcvol	400.040	ml/mol	McGowan Method
pc	773.75	kPa	Joback Method
rinpol	3203.00		NIST Webbook
rinpol	3203.00		NIST Webbook
tb	1027.36	K	Joback Method
tc	1268.40	K	Joback Method
tf	587.28	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.44	J/mol×K	1027.36	Joback Method
cpg	1400.54	J/mol×K	1067.53	Joback Method
cpg	1416.71	J/mol×K	1107.71	Joback Method
cpg	1431.04	J/mol×K	1147.88	Joback Method
cpg	1443.59	J/mol×K	1188.05	Joback Method
cpg	1454.43	J/mol×K	1228.22	Joback Method
cpg	1463.63	J/mol×K	1268.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377260&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