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

Inchi: InChI=1S/C31H50F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25-36-29(34)23-2

InchiKey: SKZZCSUPKKOACJ-UHFFFAOYSA-N

Formula: C31H50F2O4

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

Mol. weight [g/mol]: 524.72

Physical Properties

Property code	Value	Unit	Source
gf	-556.61	kJ/mol	Joback Method
hf	-1356.68	kJ/mol	Joback Method
hfus	77.52	kJ/mol	Joback Method
hvap	104.49	kJ/mol	Joback Method
log10ws	-10.75		Crippen Method
logp	9.544		Crippen Method
mcvol	442.310	ml/mol	McGowan Method
pc	663.23	kPa	Joback Method
rinpol	3510.00		NIST Webbook
rinpol	3510.00		NIST Webbook
tb	1096.00	K	Joback Method
tc	1374.51	K	Joback Method
tf	621.09	K	Joback Method
vc	1.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.79	J/mol×K	1096.00	Joback Method
cpg	1592.29	J/mol×K	1142.42	Joback Method
cpg	1609.23	J/mol×K	1188.84	Joback Method
cpg	1623.74	J/mol×K	1235.26	Joback Method
cpg	1635.95	J/mol×K	1281.67	Joback Method
cpg	1645.99	J/mol×K	1328.09	Joback Method
cpg	1653.98	J/mol×K	1374.51	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=U377263&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