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

Inchi: InChI=1S/C24H36F2O4/c1-3-4-5-6-7-8-9-10-11-18-29-22(27)16-13-17-23(28)30-19(2)24

InchiKey: BUTYVOWWRXQNBT-UHFFFAOYSA-N

Formula: C24H36F2O4

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

Mol. weight [g/mol]: 426.54

Physical Properties

Property code	Value	Unit	Source
gf	-615.55	kJ/mol	Joback Method
hf	-1212.20	kJ/mol	Joback Method
hfus	59.39	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.813		Crippen Method
mcvol	343.680	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2791.00		NIST Webbook
tb	935.84	K	Joback Method
tc	1145.80	K	Joback Method
tf	542.20	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.26	J/mol×K	935.84	Joback Method
cpg	1149.86	J/mol×K	970.83	Joback Method
cpg	1165.06	J/mol×K	1005.83	Joback Method
cpg	1178.91	J/mol×K	1040.82	Joback Method
cpg	1191.43	J/mol×K	1075.81	Joback Method
cpg	1202.67	J/mol×K	1110.81	Joback Method
cpg	1212.65	J/mol×K	1145.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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