Phthalic acid, 1-(2,6-difluorophenyl)ethyl tridecyl ester

Inchi: InChI=1S/C29H38F2O4/c1-3-4-5-6-7-8-9-10-11-12-15-21-34-28(32)23-17-13-14-18-24(2

InchiKey: OGIMVSAYKFNGRA-UHFFFAOYSA-N

Formula: C29H38F2O4

SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 488.61

Physical Properties

Property code	Value	Unit	Source
gf	-470.67	kJ/mol	Joback Method
hf	-1090.34	kJ/mol	Joback Method
hfus	65.99	kJ/mol	Joback Method
hvap	102.98	kJ/mol	Joback Method
log10ws	-10.13		Crippen Method
logp	8.351		Crippen Method
mcvol	390.370	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	3248.00		NIST Webbook
rinpol	3248.00		NIST Webbook
tb	1081.90	K	Joback Method
tc	1328.55	K	Joback Method
tf	637.49	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1333.17	J/mol×K	1081.90	Joback Method
cpg	1347.43	J/mol×K	1123.01	Joback Method
cpg	1359.85	J/mol×K	1164.12	Joback Method
cpg	1370.53	J/mol×K	1205.23	Joback Method
cpg	1379.54	J/mol×K	1246.33	Joback Method
cpg	1386.96	J/mol×K	1287.44	Joback Method
cpg	1392.88	J/mol×K	1328.55	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=U377754&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