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

Inchi: InChI=1S/C27H34F2O4/c1-3-4-5-6-7-8-9-10-13-19-32-26(30)21-15-11-12-16-22(21)27(3

InchiKey: CGSKBXNSKXAQIL-UHFFFAOYSA-N

Formula: C27H34F2O4

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

Mol. weight [g/mol]: 460.55

Physical Properties

Property code	Value	Unit	Source
gf	-487.51	kJ/mol	Joback Method
hf	-1049.06	kJ/mol	Joback Method
hfus	60.81	kJ/mol	Joback Method
hvap	98.52	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	7.570		Crippen Method
mcvol	362.190	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	3988.00		NIST Webbook
rinpol	3988.00		NIST Webbook
tb	1036.14	K	Joback Method
tc	1268.74	K	Joback Method
tf	614.95	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.34	J/mol×K	1036.14	Joback Method
cpg	1224.30	J/mol×K	1074.91	Joback Method
cpg	1236.64	J/mol×K	1113.67	Joback Method
cpg	1247.43	J/mol×K	1152.44	Joback Method
cpg	1256.72	J/mol×K	1191.21	Joback Method
cpg	1264.58	J/mol×K	1229.98	Joback Method
cpg	1271.06	J/mol×K	1268.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377768&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

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

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