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

Inchi: InChI=1S/C28H36F2O4/c1-3-4-5-6-7-8-9-10-11-14-20-33-27(31)22-16-12-13-17-23(22)2

InchiKey: ASOYNBUWHBOLEZ-UHFFFAOYSA-N

Formula: C28H36F2O4

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

Mol. weight [g/mol]: 474.58

Physical Properties

Property code	Value	Unit	Source
gf	-479.09	kJ/mol	Joback Method
hf	-1069.70	kJ/mol	Joback Method
hfus	63.40	kJ/mol	Joback Method
hvap	100.75	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	7.960		Crippen Method
mcvol	376.280	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	3140.00		NIST Webbook
tb	1059.02	K	Joback Method
tc	1298.04	K	Joback Method
tf	626.22	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1271.60	J/mol×K	1059.02	Joback Method
cpg	1285.69	J/mol×K	1098.86	Joback Method
cpg	1298.08	J/mol×K	1138.69	Joback Method
cpg	1308.82	J/mol×K	1178.53	Joback Method
cpg	1317.98	J/mol×K	1218.36	Joback Method
cpg	1325.64	J/mol×K	1258.20	Joback Method
cpg	1331.86	J/mol×K	1298.04	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=U377766&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