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

Inchi: InChI=1S/C25H30F2O4/c1-3-4-5-6-7-8-11-17-30-24(28)19-13-9-10-14-20(19)25(29)31-1

InchiKey: WOQKOLBZJFXOPQ-UHFFFAOYSA-N

Formula: C25H30F2O4

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

Mol. weight [g/mol]: 432.50

Physical Properties

Property code	Value	Unit	Source
gf	-504.35	kJ/mol	Joback Method
hf	-1007.78	kJ/mol	Joback Method
hfus	55.63	kJ/mol	Joback Method
hvap	94.07	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	6.790		Crippen Method
mcvol	334.010	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	990.38	K	Joback Method
tc	1213.51	K	Joback Method
tf	592.41	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.96	J/mol×K	990.38	Joback Method
cpg	1102.67	J/mol×K	1027.57	Joback Method
cpg	1114.93	J/mol×K	1064.76	Joback Method
cpg	1125.79	J/mol×K	1101.94	Joback Method
cpg	1135.28	J/mol×K	1139.13	Joback Method
cpg	1143.45	J/mol×K	1176.32	Joback Method
cpg	1150.35	J/mol×K	1213.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377796&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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