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

Inchi: InChI=1S/C26H32F2O4/c1-3-4-5-6-7-8-9-12-18-31-25(29)20-14-10-11-15-21(20)26(30)3

InchiKey: RBPAGCOIWDPTKH-UHFFFAOYSA-N

Formula: C26H32F2O4

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

Mol. weight [g/mol]: 446.53

Physical Properties

Property code	Value	Unit	Source
gf	-495.93	kJ/mol	Joback Method
hf	-1028.42	kJ/mol	Joback Method
hfus	58.22	kJ/mol	Joback Method
hvap	96.30	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	7.180		Crippen Method
mcvol	348.100	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2937.00		NIST Webbook
rinpol	2937.00		NIST Webbook
tb	1013.26	K	Joback Method
tc	1240.59	K	Joback Method
tf	603.68	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.45	J/mol×K	1013.26	Joback Method
cpg	1163.28	J/mol×K	1051.15	Joback Method
cpg	1175.58	J/mol×K	1089.04	Joback Method
cpg	1186.41	J/mol×K	1126.93	Joback Method
cpg	1195.81	J/mol×K	1164.81	Joback Method
cpg	1203.84	J/mol×K	1202.70	Joback Method
cpg	1210.55	J/mol×K	1240.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377786&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