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

Inchi: InChI=1S/C22H24F2O4/c1-3-4-5-8-14-27-21(25)16-10-6-7-11-17(16)22(26)28-15(2)20-1

InchiKey: PIHPZRHOFCPCCY-UHFFFAOYSA-N

Formula: C22H24F2O4

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

Mol. weight [g/mol]: 390.42

Physical Properties

Property code	Value	Unit	Source
gf	-529.61	kJ/mol	Joback Method
hf	-945.86	kJ/mol	Joback Method
hfus	47.86	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.620		Crippen Method
mcvol	291.740	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook
tb	921.74	K	Joback Method
tc	1138.00	K	Joback Method
tf	558.60	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.41	J/mol×K	921.74	Joback Method
cpg	923.81	J/mol×K	957.78	Joback Method
cpg	935.93	J/mol×K	993.83	Joback Method
cpg	946.79	J/mol×K	1029.87	Joback Method
cpg	956.42	J/mol×K	1065.91	Joback Method
cpg	964.87	J/mol×K	1101.95	Joback Method
cpg	972.15	J/mol×K	1138.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377798&Units=SI

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