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

Inchi: InChI=1S/C23H26F2O4/c1-3-4-5-6-9-15-28-22(26)17-11-7-8-12-18(17)23(27)29-16(2)21

InchiKey: WBSDWFTXCWYSGS-UHFFFAOYSA-N

Formula: C23H26F2O4

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

Mol. weight [g/mol]: 404.45

Physical Properties

Property code	Value	Unit	Source
gf	-521.19	kJ/mol	Joback Method
hf	-966.50	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	89.62	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	6.010		Crippen Method
mcvol	305.830	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2639.00		NIST Webbook
tb	944.62	K	Joback Method
tc	1162.27	K	Joback Method
tf	569.87	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.39	J/mol×K	944.62	Joback Method
cpg	982.89	J/mol×K	980.90	Joback Method
cpg	995.06	J/mol×K	1017.17	Joback Method
cpg	1005.94	J/mol×K	1053.45	Joback Method
cpg	1015.55	J/mol×K	1089.72	Joback Method
cpg	1023.93	J/mol×K	1126.00	Joback Method
cpg	1031.11	J/mol×K	1162.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377797&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