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

Inchi: InChI=1S/C24H18F4O4/c1-13(21-17(25)9-5-10-18(21)26)31-23(29)15-7-3-4-8-16(15)24(

InchiKey: KRWHDSPXQWRLTL-UHFFFAOYSA-N

Formula: C24H18F4O4

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

Mol. weight [g/mol]: 446.39

Physical Properties

Property code	Value	Unit	Source
gf	-811.68	kJ/mol	Joback Method
hf	-1171.05	kJ/mol	Joback Method
hfus	48.94	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.079		Crippen Method
mcvol	299.700	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2733.00		NIST Webbook
tb	1002.24	K	Joback Method
tc	1234.66	K	Joback Method
tf	618.78	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	931.76	J/mol×K	1002.24	Joback Method
cpg	941.83	J/mol×K	1040.98	Joback Method
cpg	950.46	J/mol×K	1079.71	Joback Method
cpg	957.71	J/mol×K	1118.45	Joback Method
cpg	963.60	J/mol×K	1157.19	Joback Method
cpg	968.19	J/mol×K	1195.93	Joback Method
cpg	971.51	J/mol×K	1234.66	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=U377722&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