Isophthalic acid, 2-fluorophenyl pentadecyl ester

Inchi: InChI=1S/C29H39FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-22-33-28(31)24-18-17-19-25(2

InchiKey: UYUGOYUPLINPMO-UHFFFAOYSA-N

Formula: C29H39FO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2F)c1

Mol. weight [g/mol]: 470.62

Physical Properties

Property code	Value	Unit	Source
gf	-263.79	kJ/mol	Joback Method
hf	-877.48	kJ/mol	Joback Method
hfus	66.82	kJ/mol	Joback Method
hvap	103.52	kJ/mol	Joback Method
log10ws	-9.99		Crippen Method
logp	8.293		Crippen Method
mcvol	388.600	ml/mol	McGowan Method
pc	905.61	kPa	Joback Method
rinpol	3622.00		NIST Webbook
rinpol	3622.00		NIST Webbook
tb	1078.09	K	Joback Method
tc	1322.44	K	Joback Method
tf	639.38	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1327.76	J/mol×K	1078.09	Joback Method
cpg	1342.44	J/mol×K	1118.81	Joback Method
cpg	1355.38	J/mol×K	1159.54	Joback Method
cpg	1366.66	J/mol×K	1200.26	Joback Method
cpg	1376.38	J/mol×K	1240.99	Joback Method
cpg	1384.62	J/mol×K	1281.71	Joback Method
cpg	1391.47	J/mol×K	1322.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344663&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