Isophthalic acid, 2-fluorophenyl tetradecyl ester

Inchi: InChI=1S/C28H37FO4/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-32-27(30)23-17-16-18-24(22-2

InchiKey: DQYDVZQRAQYTON-UHFFFAOYSA-N

Formula: C28H37FO4

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

Mol. weight [g/mol]: 456.59

Physical Properties

Property code	Value	Unit	Source
gf	-272.21	kJ/mol	Joback Method
hf	-856.84	kJ/mol	Joback Method
hfus	64.23	kJ/mol	Joback Method
hvap	101.29	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	7.903		Crippen Method
mcvol	374.510	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
tb	1055.21	K	Joback Method
tc	1292.56	K	Joback Method
tf	628.11	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.98	J/mol×K	1055.21	Joback Method
cpg	1280.48	J/mol×K	1094.77	Joback Method
cpg	1293.34	J/mol×K	1134.33	Joback Method
cpg	1304.64	J/mol×K	1173.88	Joback Method
cpg	1314.44	J/mol×K	1213.44	Joback Method
cpg	1322.83	J/mol×K	1253.00	Joback Method
cpg	1329.88	J/mol×K	1292.56	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=U344662&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume