Isophthalic acid, 2-fluorophenyl undecyl ester

Inchi: InChI=1S/C25H31FO4/c1-2-3-4-5-6-7-8-9-12-18-29-24(27)20-14-13-15-21(19-20)25(28)3
InchiKey: WEBAQRQSVHWHSG-UHFFFAOYSA-N
Formula: C25H31FO4
SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2F)c1
Mol. weight [g/mol]: 414.51

Physical Properties

Property code	Value	Unit	Source
gf	-297.47	kJ/mol	Joback Method
hf	-794.92	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	94.61	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	6.732		Crippen Method
mcvol	332.240	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	3183.00		NIST Webbook
rinpol	3183.00		NIST Webbook
tb	986.57	K	Joback Method
tc	1209.75	K	Joback Method
tf	594.30	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1082.82	J/mol×K	986.57	Joback Method
cpg	1096.93	J/mol×K	1023.77	Joback Method
cpg	1109.61	J/mol×K	1060.96	Joback Method
cpg	1120.93	J/mol×K	1098.16	Joback Method
cpg	1130.93	J/mol×K	1135.35	Joback Method
cpg	1139.66	J/mol×K	1172.55	Joback Method
cpg	1147.18	J/mol×K	1209.75	Joback Method

Sources

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=U344660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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