Isophthalic acid, 3,5-difluorophenyl undecyl ester

Inchi: InChI=1S/C25H30F2O4/c1-2-3-4-5-6-7-8-9-10-14-30-24(28)19-12-11-13-20(15-19)25(29

InchiKey: IGVZQJLSPKUZFD-UHFFFAOYSA-N

Formula: C25H30F2O4

SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1

Mol. weight [g/mol]: 432.50

Physical Properties

Property code	Value	Unit	Source
gf	-501.91	kJ/mol	Joback Method
hf	-1002.50	kJ/mol	Joback Method
hfus	59.15	kJ/mol	Joback Method
hvap	94.46	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	6.872		Crippen Method
mcvol	334.010	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
tb	990.82	K	Joback Method
tc	1213.56	K	Joback Method
tf	607.41	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.57	J/mol×K	990.82	Joback Method
cpg	1102.32	J/mol×K	1027.94	Joback Method
cpg	1114.64	J/mol×K	1065.07	Joback Method
cpg	1125.57	J/mol×K	1102.19	Joback Method
cpg	1135.15	J/mol×K	1139.31	Joback Method
cpg	1143.44	J/mol×K	1176.44	Joback Method
cpg	1150.47	J/mol×K	1213.56	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=U344378&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume