Isophthalic acid, 3,5-difluorophenyl dodecyl ester

Inchi: InChI=1S/C26H32F2O4/c1-2-3-4-5-6-7-8-9-10-11-15-31-25(29)20-13-12-14-21(16-20)26

InchiKey: ZGKXHRKLZBOLLT-UHFFFAOYSA-N

Formula: C26H32F2O4

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

Mol. weight [g/mol]: 446.53

Physical Properties

Property code	Value	Unit	Source
gf	-493.49	kJ/mol	Joback Method
hf	-1023.14	kJ/mol	Joback Method
hfus	61.74	kJ/mol	Joback Method
hvap	96.69	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	7.262		Crippen Method
mcvol	348.100	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	3195.00		NIST Webbook
tb	1013.70	K	Joback Method
tc	1241.05	K	Joback Method
tf	618.68	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.11	J/mol×K	1013.70	Joback Method
cpg	1163.01	J/mol×K	1051.59	Joback Method
cpg	1175.39	J/mol×K	1089.48	Joback Method
cpg	1186.32	J/mol×K	1127.38	Joback Method
cpg	1195.83	J/mol×K	1165.27	Joback Method
cpg	1203.99	J/mol×K	1203.16	Joback Method
cpg	1210.84	J/mol×K	1241.05	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=U344379&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