Isophthalic acid, 3,5-difluorophenyl decyl ester

Inchi: InChI=1S/C24H28F2O4/c1-2-3-4-5-6-7-8-9-13-29-23(27)18-11-10-12-19(14-18)24(28)30

InchiKey: OSOYDPGHCHPSOZ-UHFFFAOYSA-N

Formula: C24H28F2O4

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

Mol. weight [g/mol]: 418.47

Physical Properties

Property code	Value	Unit	Source
gf	-510.33	kJ/mol	Joback Method
hf	-981.86	kJ/mol	Joback Method
hfus	56.56	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	6.481		Crippen Method
mcvol	319.920	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	967.94	K	Joback Method
tc	1187.08	K	Joback Method
tf	596.14	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.50	J/mol×K	967.94	Joback Method
cpg	1042.11	J/mol×K	1004.46	Joback Method
cpg	1054.36	J/mol×K	1040.99	Joback Method
cpg	1065.28	J/mol×K	1077.51	Joback Method
cpg	1074.91	J/mol×K	1114.04	Joback Method
cpg	1083.29	J/mol×K	1150.56	Joback Method
cpg	1090.47	J/mol×K	1187.08	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=U344377&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