Isophthalic acid, 3,5-difluorophenyl pentadecyl ester

Inchi: InChI=1S/C29H38F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-34-28(32)23-16-15-17-24

InchiKey: MEABUHUEEOJIGR-UHFFFAOYSA-N

Formula: C29H38F2O4

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

Mol. weight [g/mol]: 488.61

Physical Properties

Property code	Value	Unit	Source
gf	-468.23	kJ/mol	Joback Method
hf	-1085.06	kJ/mol	Joback Method
hfus	69.52	kJ/mol	Joback Method
hvap	103.36	kJ/mol	Joback Method
log10ws	-10.32		Crippen Method
logp	8.432		Crippen Method
mcvol	390.370	ml/mol	McGowan Method
pc	873.77	kPa	Joback Method
rinpol	3526.00		NIST Webbook
rinpol	3526.00		NIST Webbook
tb	1082.34	K	Joback Method
tc	1330.36	K	Joback Method
tf	652.49	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.99	J/mol×K	1082.34	Joback Method
cpg	1347.42	J/mol×K	1123.68	Joback Method
cpg	1360.02	J/mol×K	1165.01	Joback Method
cpg	1370.87	J/mol×K	1206.35	Joback Method
cpg	1380.06	J/mol×K	1247.69	Joback Method
cpg	1387.66	J/mol×K	1289.02	Joback Method
cpg	1393.76	J/mol×K	1330.36	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=U344380&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