Isophthalic acid, 2,2,3,3,4,4,5,5-octafluoropentyl undecyl ester

Inchi: InChI=1S/C24H30F8O4/c1-2-3-4-5-6-7-8-9-10-14-35-19(33)17-12-11-13-18(15-17)20(34

InchiKey: BNTLORXXZITVCW-UHFFFAOYSA-N

Formula: C24H30F8O4

SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1

Mol. weight [g/mol]: 534.48

Physical Properties

Property code	Value	Unit	Source
gf	-1766.26	kJ/mol	Joback Method
hf	-2403.64	kJ/mol	Joback Method
hfus	56.02	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	7.702		Crippen Method
mcvol	354.300	ml/mol	McGowan Method
pc	860.49	kPa	Joback Method
rinpol	2572.00		NIST Webbook
rinpol	2572.00		NIST Webbook
tb	916.79	K	Joback Method
tc	1124.17	K	Joback Method
tf	540.48	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.94	J/mol×K	916.79	Joback Method
cpg	1192.49	J/mol×K	951.35	Joback Method
cpg	1206.92	J/mol×K	985.92	Joback Method
cpg	1220.31	J/mol×K	1020.48	Joback Method
cpg	1232.77	J/mol×K	1055.04	Joback Method
cpg	1244.40	J/mol×K	1089.61	Joback Method
cpg	1255.30	J/mol×K	1124.17	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=U356595&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