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

Inchi: InChI=1S/C30H42F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-41-25(39)23-18-17

InchiKey: GAXDXSKGNONBRZ-UHFFFAOYSA-N

Formula: C30H42F8O4

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

Mol. weight [g/mol]: 618.64

Physical Properties

Property code	Value	Unit	Source
gf	-1715.74	kJ/mol	Joback Method
hf	-2527.48	kJ/mol	Joback Method
hfus	71.56	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-11.58		Crippen Method
logp	10.043		Crippen Method
mcvol	438.840	ml/mol	McGowan Method
pc	629.71	kPa	Joback Method
rinpol	3163.00		NIST Webbook
tb	1054.07	K	Joback Method
tc	1326.63	K	Joback Method
tf	608.10	K	Joback Method
vc	1.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.76	J/mol×K	1054.07	Joback Method
cpg	1569.17	J/mol×K	1099.50	Joback Method
cpg	1587.99	J/mol×K	1144.92	Joback Method
cpg	1605.50	J/mol×K	1190.35	Joback Method
cpg	1621.96	J/mol×K	1235.78	Joback Method
cpg	1637.65	J/mol×K	1281.21	Joback Method
cpg	1652.83	J/mol×K	1326.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356601&Units=SI
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

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