Isophthalic acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

Inchi: InChI=1S/C18H10F16O4/c19-11(20)15(27,28)17(31,32)13(23,24)5-37-9(35)7-2-1-3-8(4-7)10(36)38-6-14(25,26)18(33,34)16(29,30)12(21)22/h1-4,11-12H,5-6H2

InchiKey: NYOUDFDPEYLGEO-UHFFFAOYSA-N

Formula: C18H10F16O4

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

Mol. weight [g/mol]: 594.24

Physical Properties

Property code	Value	Unit	Source
gf	-3369.18	kJ/mol	Joback Method
hf	-3880.21	kJ/mol	Joback Method
hfus	39.35	kJ/mol	Joback Method
hvap	55.29	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.342		Crippen Method
mcvol	283.920	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	763.54	K	Joback Method
tc	935.40	K	Joback Method
tf	469.84	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.73	J/mol×K	763.54	Joback Method
cpg	906.65	J/mol×K	792.18	Joback Method
cpg	916.69	J/mol×K	820.83	Joback Method
cpg	925.91	J/mol×K	849.47	Joback Method
cpg	934.41	J/mol×K	878.11	Joback Method
cpg	942.27	J/mol×K	906.76	Joback Method
cpg	949.58	J/mol×K	935.40	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=U356603&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