Cyclo-tetrakis(bis(2,2,2-trifluoroethoxy)phosphon

Inchi: InChI=1S/C16H16F24N4O8P4/c17-9(18,19)1-45-53(46-2-10(20,21)22)41-54(47-3-11(23
InchiKey: WUIXPLGUKKVBAS-UHFFFAOYSA-N
Formula: C16H16F24N4O8P4
SMILES: FC(F)(F)COP1(OCC(F)(F)F)=NP(OCC(F)(F)F)(OCC(F)(F)F)=NP(OCC(F)(F)F)(OCC(F)(F
Mol. weight [g/mol]: 972.18
CAS: 562-88-9

Physical Properties

Property code	Value	Unit	Source
ie	10.01 ± 0.05	eV	NIST Webbook
log10ws	1.56		Crippen Method
logp	12.416		Crippen Method
mcvol	436.640	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C562889&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.