Pentaerythritol, bis(cyclic hexadecyl phosphite)

Inchi: InChI=1S/C37H74O6P2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-38-44-40-33-37(3

InchiKey: NCNOFYROBGZOKR-UHFFFAOYSA-N

Formula: C37H74O6P2

SMILES: CCCCCCCCCCCCCCCCOP1OCC2(CO1)COP(OCCCCCCCCCCCCCCCC)OC2

Mol. weight [g/mol]: 676.93

CAS: 72732-57-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	13.516		Crippen Method
mcvol	586.610	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72732571&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume