

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(3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-38-44-40-33-37)P(=O)(OC1CCCCCCCCCCCCCCC)OC2(CO1)COP(OC1CCCCCCCCCCCCCCC)OC2

InchiKey: NCNOFYROBGZOKR-UHFFFAOYSA-N

Formula: C37H74O6P2

SMILES: CCCCCCCCCCCCCCCCOP1OCC2(CO1)COP(OC1CCCCCCCCCCCCCCC)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
mvol	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/ci9903071>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/88-321-8/Pentaerythritol-bis-cyclic-hexadecyl-phosphite.pdf>

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