Phosphonothioic acid, methyl-, o,o-dihexyl ester

Inchi: InChI=1S/C13H29O2PS/c1-4-6-8-10-12-14-16(3,17)15-13-11-9-7-5-2/h4-13H2,1-3H3
InchiKey: CMLHRUBXPKTNOL-UHFFFAOYSA-N
Formula: C13H29O2PS
SMILES: CCCCCCOP(C)(=S)OCCCCCC
Mol. weight [g/mol]: 280.41
CAS: 116401-93-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	5.120		Crippen Method
mcvol	242.580	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401935&Units=SI

Legend

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

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