Phosphonothioic acid, methyl-, o,o-bis-3,3-dimethyl butyl ester

Inchi: InChI=1S/C13H29O2PS/c1-12(2,3)8-10-14-16(7,17)15-11-9-13(4,5)6/h8-11H2,1-7H3
InchiKey: YMMINPHWFMVMOD-UHFFFAOYSA-N
Formula: C13H29O2PS
SMILES: CC(C)(C)CCOP(C)(=S)OCCC(C)(C)C
Mol. weight [g/mol]: 280.41
CAS: 116401-92-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.22		Crippen Method
logp	4.831		Crippen Method
mcvol	242.580	ml/mol	McGowan Method

Sources

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=C116401924&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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