

# 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:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401924&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401924&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/116-311-7/Phosphonothioic-acid-methyl-o-o-bis-3-3-dimethyl-butyl-ester.pdf>

Generated by Cheméo on 2024-04-30 21:44:33.851642667 +0000 UTC m=+16802722.772219982.

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