Phosphonothioic acid, methyl-, o,o-diisopropyl ester

Inchi: InChI=1S/C7H17O2PS/c1-6(2)8-10(5,11)9-7(3)4/h6-7H,1-5H3
InchiKey: WJZQSIVAHFZAQJ-UHFFFAOYSA-N
Formula: C7H17O2PS
SMILES: CC(C)OP(C)(=S)OC(C)C
Mol. weight [g/mol]: 196.25
CAS: 66295-45-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.59		Crippen Method
logp	2.776		Crippen Method
mcvol	158.040	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66295452&Units=SI
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

Legend

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