Phosphonothioic acid, methyl-, o,o-dimethyl ester

Inchi: InChI=1S/C3H9O2PS/c1-4-6(3,7)5-2/h1-3H3
InchiKey: BHFOAIMSKFAWOU-UHFFFAOYSA-N
Formula: C3H9O2PS
SMILES: COP(C)(=S)OC
Mol. weight [g/mol]: 140.14
CAS: 681-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	3.48		Crippen Method
logp	1.218		Crippen Method
mcvol	101.680	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=C681061&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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