Deuterophosphonic acid, dimethyl ester

Inchi: InChI=1S/C2H7O3P/c1-4-6(3)5-2/h6H,1-2H3/i6D
InchiKey: HZCDANOFLILNSA-RAMDWTOOSA-N
Formula: C2H6DO3P
SMILES: CO[PH](=O)OC
Mol. weight [g/mol]: 111.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	0.669		Crippen Method
mcvol	77.110	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009148&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