O-Ethyl S-methyl methylphosphonothiolate

Inchi: InChI=1S/C4H11O2PS/c1-4-6-7(2,5)8-3/h4H2,1-3H3
InchiKey: RGYCUYGGOREOSJ-UHFFFAOYSA-N
Formula: C4H11O2PS
SMILES: CCOP(C)(=O)SC
Mol. weight [g/mol]: 154.17
CAS: 51865-09-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	2.209		Crippen Method
mcvol	115.770	ml/mol	McGowan Method
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51865099&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
rinpol: Non-polar retention indices

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