o-Ethyl S-2-(ethylthio)ethyl methylphosphonothiolate

Inchi: InChI=1S/C7H17O2PS2/c1-4-9-10(3,8)12-7-6-11-5-2/h4-7H2,1-3H3
InchiKey: FSBPLRBNEBOJLL-UHFFFAOYSA-N
Formula: C7H17O2PS2
SMILES: CCOP(C)(=O)SCCSCC
Mol. weight [g/mol]: 228.31
CAS: 556-75-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	3.332		Crippen Method
mcvol	174.390	ml/mol	McGowan Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C556752&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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