

O-Ethyl S-2-dimethylaminoethyl ethylphosphonothiolate

Other names: Ethyl-phosphonothioic acid S-(2-dimethylamino-ethyl) ester O-ethyl ester
Inchi: InChI=1S/C8H20NO2PS/c1-5-11-12(10,6-2)13-8-7-9(3)4/h5-8H2,1-4H3
InchiKey: LLMAYCPOBKHQIP-UHFFFAOYSA-N
Formula: C8H20NO2PS
SMILES: CCOP(=O)(CC)SCCN(C)C
Mol. weight [g/mol]: 225.29
CAS: 98543-25-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.99 | | Crippen Method |
| logp | 2.531 | | Crippen Method |
| mcvol | 182.110 | ml/mol | McGowan Method |
| rinpol | 1521.70 | | NIST Webbook |
| rinpol | 1522.00 | | NIST Webbook |
| rinpol | 1522.00 | | NIST Webbook |
| rinpol | 1521.70 | | NIST Webbook |
| rinpol | 1522.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C98543250&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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