

Methyldithiophosphonic acid, S,S-bis(2-diisopropylaminoethyl) ester

Other names: Methylthiophosphonic acid, S,S-bis-(2-diisopropylaminoethyl) ester
Inchi: InChI=1S/C17H39N2OPS2/c1-14(2)18(15(3)4)10-12-22-21(9,20)23-13-11-19(16(5)6)17(8)
InchiKey: JEWOHIVFHZQINT-UHFFFAOYSA-N
Formula: C17H39N2OPS2
SMILES: CC(C)N(CCSP(C)(=O)SCCN(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 382.61
CAS: 169493-13-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.57 | | Crippen Method |
| logp | 5.513 | | Crippen Method |
| mcvol | 329.380 | ml/mol | McGowan Method |
| rinsol | 2527.00 | | NIST Webbook |
| rinsol | 2527.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C169493134&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
rinsol: Non-polar retention indices

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