# Acephate

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|---|---|
| **Other names:** | 75 SP |
| | Acefate |
| | Acephat |
| | Acetamidophos |
| | Acetylphosphoramidothioic acid O,S-dimethyl ester |
| | Chevron RE 12,420 |
| | ENT 27822 |
| | N-(Methoxy(methylthio)phosphinoyl)acetamide |
| | O,S-Dimethyl N-acetylphosphoramidothioate |
| | O,S-Dimethyl acetylamidothiophosphate |
| | O,S-Dimethyl acetylphosphoramidothioate |
| | O,S-Dimethylacetylphosphoroamidothioate |
| | O,S-dimethyl N-acetylphosphoramidothiolate |
| | ORTHO 124120 |
| | Orthene |
| | Orthene-755 |
| | Ortran |
| | Ortril |
| | Phosphoramidothioic acid, N-acetyl-, O,S-dimethyl ester |
| | Phosphoramidothioic acid, acetyl-, O,S-dimethyl ester |
| | RE 12420 |
| **Inchi:** | InChI=1S/C4H10NO3PS/c1-4(6)5-9(7,8-2)10-3/h1-3H3,(H,5,6,7) |
| **InchiKey:** | YASYVMFAVPKPKE-UHFFFAOYSA-N |
| **Formula:** | C4H10NO3PS |
| **SMILES:** | COP(=O)(NC(C)=O)SC |
| **Mol. weight [g/mol]:** | 183.17 |
| **CAS:** | 30560-19-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | 0.54 | | Aqueous Solubility Prediction Method |
| log10ws | 0.54 | | Estimated Solubility Method |
| logp | 1.240 | | Crippen Method |
| mcvol | 127.320 | ml/mol | McGowan Method |
| rinpol | 1423.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1437.00 | | NIST Webbook |
| rinpol | 1440.00 | | NIST Webbook |
| rinpol | 1456.00 | | NIST Webbook |
| rinpol | 1452.00 | | NIST Webbook |
| rinpol | 1436.00 | | NIST Webbook |
| rinpol | 1440.00 | | NIST Webbook |
| tf | 365.10 ± 0.20 | K | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C30560191&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Solubility of Acephate in Different Solvents from (292.90 to 327.60) K:** https://www.doi.org/10.1021/je0603630

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

# Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

**tf:** Normal melting (fusion) point