

Diethyl 3-cyano-phenyl phosphate

Inchi: InChI=1S/C11H14NO4P/c1-3-14-17(13,15-4-2)16-11-7-5-6-10(8-11)9-12/h5-8H,3-4H2,1-
InchiKey: UMJPNIRIQPRRMT-UHFFFAOYSA-N
Formula: C11H14NO4P
SMILES: CCOP(=O)(OCC)Oc1cccc(C#N)c1
Mol. weight [g/mol]: 255.21

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.64 | | Crippen Method |
| logp | 3.118 | | Crippen Method |
| mcvol | 187.410 | ml/mol | McGowan Method |
| rinpol | 1780.00 | | NIST Webbook |
| rinpol | 1780.00 | | NIST Webbook |
| ripol | 2725.00 | | NIST Webbook |
| ripol | 2725.00 | | NIST Webbook |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168939&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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