

Phosphonic acid, butyl-, ethyl ester, diester with 1,4-butanediol

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|----------------------|--|
| Inchi: | InChI=1S/C16H36O6P2/c1-5-9-15-23(17,19-7-3)21-13-11-12-14-22-24(18,20-8-4)16-10- |
| InchiKey: | AGCWSTJSKCQZHB-UHFFFAOYSA-N |
| Formula: | C16H36O6P2 |
| SMILES: | CCCCP(=O)(OCC)OCCCCOP(=O)(CCCC)OCC |
| Mol. weight [g/mol]: | 386.40 |
| CAS: | 5284-06-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.42 | | Crippen Method |
| logp | 5.859 | | Crippen Method |
| mcvol | 312.440 | ml/mol | McGowan Method |

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=C5284060&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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