

1,3-Propanediol, 2,2-dimethyl-, cyclic chloromethyl phosphonate

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|-----------------------------|---|
| Inchi: | InChI=1S/C6H12ClO3P/c1-6(2)3-9-11(8,5-7)10-4-6/h3-5H2,1-2H3 |
| InchiKey: | PJRZVIMIZYGXOX-UHFFFAOYSA-N |
| Formula: | C6H12ClO3P |
| SMILES: | CC1(C)COP(=O)(CCl)OC1 |
| Mol. weight [g/mol]: | 198.58 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.08 | | Crippen Method |
| logp | 2.449 | | Crippen Method |
| mcvol | 134.850 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000931&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 |

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