

Trimethyl phosphonoacetate

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|-----------------------------|---|
| Other names: | Trimethyl phosphonacetate Acetic acid, (dimethoxyphosphinyl)-, methyl ester Methyl (dimethoxyphosphoryl)acetate |
| Inchi: | InChI=1S/C5H11O5P/c1-8-5(6)4-11(7,9-2)10-3/h4H2,1-3H3 |
| InchiKey: | SIGOIUCRXKUEIG-UHFFFAOYSA-N |
| Formula: | C5H11O5P |
| SMILES: | <chem>COC(=O)CP(=O)(OC)OC</chem> |
| Mol. weight [g/mol]: | 182.11 |
| CAS: | 5927-18-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.23 | | Crippen Method |
| logp | 0.645 | | Crippen Method |
| mcvol | 126.820 | 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=C5927184&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 |

Latest version available from:

<https://www.chemeo.com/cid/72-975-0/Trimethyl-phosphonoacetate.pdf>

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