

# Phosphonic acid, (2-chloroethyl)-, diethyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Diethyl (2-chloroethyl)phosphonate<br>Diethyl 2-chloroethanephosphonate<br>(2-Chloroethyl)phosphonic acid diethyl ester |
| <b>Inchi:</b>               | InChI=1S/C6H14ClO3P/c1-3-9-11(8,6-5-7)10-4-2/h3-6H2,1-2H3   |
| <b>InchiKey:</b>            | GMDLEOVIACJWTD-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C6H14ClO3P  |
| <b>SMILES:</b>              | CCOP(=O)(CCCl)OCC   |
| <b>Mol. weight [g/mol]:</b> | 200.60  |
| <b>CAS:</b>                 | 10419-79-1  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.94   |        | Crippen Method |
| logp          | 2.491   |        | Crippen Method |
| mcvol         | 145.710 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10419791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10419791&amp;Units=SI</a> |

## Legend

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

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