

# DIMETHYL PHENYLPHOSPHONATE

|                      |                                                                              |
|----------------------|------------------------------------------------------------------------------|
| Other names:         | Phosphonic acid, phenyl-, dimethyl ester<br>O,O-Dimethyl benzene phosphonate |
| Inchi:               | InChI=1S/C8H11O3P/c1-10-12(9,11-2)8-6-4-3-5-7-8/h3-7H,1-2H3                  |
| InchiKey:            | OXDOANYFRLHSML-UHFFFAOYSA-N                                                  |
| Formula:             | C8H11O3P                                                                     |
| SMILES:              | COP(=O)(OC)c1ccccc1                                                          |
| Mol. weight [g/mol]: | 186.15                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 9.45    | eV     | Cheméo Relay (1.0) |
| logp          | 1.798   |        | Crippen Method     |
| mcvol         | 137.890 | ml/mol | McGowan Method     |
| tf            | 291.15  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Cheméo Relay (1.0):       |                                                                                                                                             |
| Cheméo Relay (1.0, beta): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2240417&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2240417&amp;Units=SI</a> |

## Legend

|        |                                     |
|--------|-------------------------------------|
| ie:    | Ionization energy                   |
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |
| tf:    | Normal melting (fusion) point       |

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