# Diethyl methylphosphonathioate

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|---|---|
| **Other names:** | Diethyl methylphosphonothionate |
| | Diethyl phosphonothioate |
| | Methylthiophosphonic acid, O,O-diethyl ester |
| | O,O'-Diethyl methylphosphonothioate |
| | O,O-Diethyl methylphosphonothioate |
| | Phosphonothioic acid, methyl-, O,O-diethyl ester |
| **Inchi:** | InChI=1S/C5H13O2PS/c1-4-6-8(3,9)7-5-2/h4-5H2,1-3H3 |
| **InchiKey:** | GEDUXIUTPVHAAV-UHFFFAOYSA-N |
| **Formula:** | C5H13O2PS |
| **SMILES:** | CCOP(C)(=S)OCC |
| **Mol. weight [g/mol]:** | 168.20 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hvap | 58.13 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.64 | eV | Cheméo Relay (1.0) |
| log10ws | -2.36 | | Cheméo Relay (1.0) |
| logp | 1.999 | | Crippen Method |
| mcvol | 129.860 | ml/mol | McGowan Method |
| tb | 487.88 | K | Cheméo Relay (1.0) |
| tf | 226.84 | K | Cheméo Relay (1.0) |

## Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6996812&Units=SI

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

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|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |