# Demeton-O

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|---|---|
| **Other names:** | Demethon-O |
| | Demeton thiono |
| | Demeton-O |
| | Demetonthione |
| | Di-Septon |
| | Diaethylthiophosphorsaeureester des aethylthioglykol |
| | Diethyl (2-(ethhthio)ethyl) thionophosphate |
| | Diethyl (2-(ethylthio)ethyl) phosphorothionate |
| | Ethanol, 2-(ethylthio)-, O-ester with O,O-diethyl phosphorothioate |
| | NSC 8928 |
| | O,O-Diethyl O-2-(ethylthio)ethyl phosphorothioate |
| | O,O-Diethyl O-[2-(ethylthio)ethyl] phosphorothionate |
| | O,O-diethyl-O-[2-(ethylthio)ethyl] thiophosphate |
| | Phosphorothioic acid, O,O-diethyl ester O-[2-(ethylthio)ethyl] ester |
| | Thiolmecaptophos |
| **Inchi:** | InChI=1S/C8H19O3PS2/c1-4-9-12(13,10-5-2)11-7-8-14-6-3/h4-8H2,1-3H3 |
| **InchiKey:** | DGLIBALSRMUQDD-UHFFFAOYSA-N |
| **Formula:** | C8H19O3PS2 |
| **SMILES:** | CCOP(=S)(OCC)OCCSCC |
| **Mol. weight [g/mol]:** | 258.35 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hvap | 78.70 | kJ/mol | NIST Webbook |
| ie | 8.50 | eV | Cheméo Relay (1.0) |
| log10ws | -3.31 | | Cheméo Relay (1.0) |
| logp | 3.054 | | Crippen Method |
| mcvol | 194.350 | ml/mol | McGowan Method |
| rinpol | 1598.00 | | NIST Webbook |
| rinpol | 1621.00 | | NIST Webbook |

# Sources

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

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C298033&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **rinpol:** | Non-polar retention indices |