# Chlorthion

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|---|---|
| **Other names:** | BAY 22190 |
| | Bayer 22/190 |
| | Chloorthion |
| | Chlorothion |
| | Chlorthion Methyl |
| | Chlortion |
| | Compound 22/190 |
| | Dimethyl 3-chloro-4-nitrophenyl thionophosphate |
| | ENT 18,861 |
| | Methyl chlorothion |
| | NSC 8927 |
| | O,O-Dimethyl O-(3-chloro-4-nitrophenyl) phosphorothioate |
| | O,O-Dimethyl O-(3-chloro-4-nitrophenyl) thiophosphate |
| | O,O-Dimethyl O-4-nitro-3-chlorophenyl thiophosphate |
| | O,O-Dimethyl p-nitro-m-chlorophenyl thiophosphate |
| | O,O-Dimethyl-O-(3-chlor-4-nitrophenyl)-monothiophosphat |
| | O,O-Dimethyl-O-(4-nitro-5-chlorphenyl)-thionophosphat |
| | O,O-Dimethyl-O-3-chlor-4-nitrofenylester kyseliny thiofosforecne |
| | O,O-Dimethyl-O-3-chlor-4-nitrofenyltiofosfat |
| | O-(3-Chloor-4-nitro-fenyl)-O,O-dimethyl-monothiofosfaat |
| | O-(3-Chlor-4-nitro-phenyl)-O,O-dimethyl-monothiophosphat |
| | O-(3-Chloro-4-nitro-fenyl)-O,O-dimethyl-monothiofosfaat |
| | O-(3-Chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate |
| | O-(3-Cloro-4-nitro-fenil)-O,O-dimetil-monotiofosfato |
| | O-(3-chloro-4-nitrophenyl) O,O-dimethyl thiophosphate |
| | OMS 217 |
| | Phenol, 3-chloro-4-nitro-, O-ester with O,O-dimethyl phosphorothioate |
| | Phosphorothioic acid, O-(3-chloro-4-nitrophenyl) O,O-dimethyl ester |
| | Thiophosphate de O,O-dimethyle et de O-3-chloro-4-nitrophenyle |
| | p-Nitro-m-chlorophenyl dimethyl thionophosphate |
| **Inchi:** | InChI=1S/C8H9ClNO5PS/c1-13-16(17,14-2)15-6-3-4-8(10(11)12)7(9)5-6/h3-5H,1-2H3 |
| **InchiKey:** | NZNRRXXETLSZRO-UHFFFAOYSA-N |
| **Formula:** | C8H9ClNO5PS |
| **SMILES:** | COP(=S)(OC)Oc1ccc([N+](=O)[O-])c(Cl)c1 |
| **Mol. weight [g/mol]:** | 297.65 |
| **CAS:** | 500-28-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | 0.23 | | Crippen Method |
| logp | 3.144 | | Crippen Method |
| mcvol | 183.900 | ml/mol | McGowan Method |
| rinpol | 1945.00 | | NIST Webbook |
| rinpol | 1964.00 | | NIST Webbook |
| rinpol | 1991.00 | | NIST Webbook |
| rinpol | 1945.00 | | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hvapt | 92.00 | kJ/mol | 346.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 2.35129e+01 |
| Coeff. B | -1.10704e+04 |
| Temperature range (K), min. | 476.65 |
| Temperature range (K), max. | 608.22 |

# Sources

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C500287&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

# Legend

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|---|---|
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |