

# Hexaethyl tetraphosphate

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H30O13P4/c1-7-17-26(13,18-8-2)23-28(15,21-11-5)25-29(16,22-12-6)24-2 |
| InchiKey:            | DAJYZXUXDOSMCG-UHFFFAOYSA-N                                                      |
| Formula:             | C12H30O13P4                                                                      |
| SMILES:              | CCOP(=O)(OCC)OP(=O)(OCC)OP(=O)(OCC)OP(=O)(OCC)OCC                                |
| Mol. weight [g/mol]: | 506.25                                                                           |
| CAS:                 | 757-58-4                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source                                                     |
|---------------|---------|--------|------------------------------------------------------------|
| hvap          | 115.27  | kJ/mol | Cheméo Relay (1.0)                                         |
| ie            | 9.82    | eV     | Cheméo Relay (1.0)                                         |
| log10ws       | -2.70   |        | Cheméo Relay (1.0)                                         |
| logp          | 5.688   |        | Crippen Method                                             |
| mcvol         | 338.090 | ml/mol | McGowan Method                                             |
| tb            | 671.00  | K      | Cheméo Relay (1.0)                                         |
| tf            | 233.15  | K      | Jean-Claude Bradley Open Melting Point Dataset (2014, CC0) |

## 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):                                   |                                                                                                                                                                                         |
| Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): | <a href="https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637">https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637</a> |

## Legend

|       |                                                 |
|-------|-------------------------------------------------|
| hvap: | Enthalpy of vaporization at standard conditions |
| ie:   | Ionization energy                               |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tf:</b>      | Normal melting (fusion) point       |

Latest version available from:

<https://www.cheméo.com/cid/108-263-0/Hexaethyl-tetraphosphate.pdf>

Generated by Cheméo on 2026-10-31 00:36:09.218502933 +0000 UTC m=+30682.145340244.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.