

# Hexaethylphosphoric triamide

|                      |                                                                              |
|----------------------|------------------------------------------------------------------------------|
| Other names:         | ((C2H5)2N)3P=O<br>OP(N(C2H5)2)3                                              |
| Inchi:               | InChI=1S/C12H30N3OP/c1-7-13(8-2)17(16,14(9-3)10-4)15(11-5)12-6/h7-12H2,1-6H3 |
| InchiKey:            | ROZPNEGZBIUWBX-UHFFFAOYSA-N                                                  |
| Formula:             | C12H30N3OP                                                                   |
| SMILES:              | CCN(CC)P(=O)(N(CC)CC)N(CC)CC                                                 |
| Mol. weight [g/mol]: | 263.36                                                                       |
| CAS:                 | 2622-07-3                                                                    |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| affp          | 974.70  | kJ/mol | NIST Webbook   |
| basg          | 942.20  | kJ/mol | NIST Webbook   |
| log10ws       | -3.82   |        | Crippen Method |
| logp          | 3.120   |        | Crippen Method |
| mcvol         | 236.210 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2622073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2622073&amp;Units=SI</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>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|          |                                     |
|----------|-------------------------------------|
| affp:    | Proton affinity                     |
| basg:    | Gas basicity                        |
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |

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