

# tri-4-Tolyl thiophosphate

|                      |                                                                                     |
|----------------------|-------------------------------------------------------------------------------------|
| Other names:         | tri-p-Tolyl thiophosphate<br>Phosphorothioic acid, O,O,O-tris(4-methylphenyl) ester |
| Inchi:               | InChI=1S/C21H21O3PS/c1-16-4-10-19(11-5-16)22-25(26,23-20-12-6-17(2)7-13-20)24-2     |
| InchiKey:            | KOPAJQQYQQKYEG-UHFFFAOYSA-N                                                         |
| Formula:             | C21H21O3PS                                                                          |
| SMILES:              | Cc1ccc(OP(=S)(Oc2ccc(C)cc2)Oc2ccc(C)cc2)cc1                                         |
| Mol. weight [g/mol]: | 384.43                                                                              |
| CAS:                 | 597-84-2                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.55   |        | Crippen Method |
| logp          | 6.373   |        | Crippen Method |
| mcvol         | 289.890 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C597842&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C597842&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

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |

Latest version available from:

<https://www.chemeo.com/cid/96-217-5/tri-4-Tolyl-thiophosphate.pdf>

Generated by Cheméo on 2025-12-05 15:45:26.036629608 +0000 UTC m=+4697723.566670285.

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