

# Phosphine, tris[4-(trifluoromethyl)phenyl]-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Phosphine, tris(«alpha», «alpha», «alpha»-trifluoro-p-tolyl)-<br>Tris[(p-trifluoromethyl)phenyl]phosphine |
| <b>Inchi:</b>               | InChI=1S/C21H12F9P/c22-19(23,24)13-1-7-16(8-2-13)31(17-9-3-14(4-10-17)20(25,26)2                          |
| <b>InchiKey:</b>            | PXYCJKZSCDFXLR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C21H12F9P   |
| <b>SMILES:</b>              | FC(F)(F)c1ccc(P(c2ccc(C(F)(F)F)cc2)c2ccc(C(F)(F)F)cc2)cc1   |
| <b>Mol. weight [g/mol]:</b> | 466.28  |
| <b>CAS:</b>                 | 13406-29-6  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -16.99  |        | Crippen Method |
| logp          | 6.501   |        | Crippen Method |
| mcvol         | 271.860 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13406296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13406296&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |

## Legend

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

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