

# Phosphine oxide, tripropyl-

|                      |                                                                                                              |
|----------------------|--------------------------------------------------------------------------------------------------------------|
| Other names:         | Phosphine oxide, tripropyl-<br>Tripropylphosphine oxide<br>OP(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> |
| Inchi:               | InChI=1S/C <sub>9</sub> H <sub>21</sub> OP/c1-4-7-11(10,8-5-2)9-6-3/h4-9H <sub>2</sub> ,1-3H <sub>3</sub>    |
| InchiKey:            | SNZSAFILJOCMFM-UHFFFAOYSA-N                                                                                  |
| Formula:             | C <sub>9</sub> H <sub>21</sub> OP                                                                            |
| SMILES:              | CCCP(=O)(CCC)CCC                                                                                             |
| Mol. weight [g/mol]: | 176.24                                                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| affp          | 948.20  | kJ/mol | NIST Webbook   |
| basg          | 918.40  | kJ/mol | NIST Webbook   |
| logp          | 3.580   |        | Crippen Method |
| mcvol         | 164.000 | ml/mol | McGowan Method |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 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): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1496942&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1496942&amp;Units=SI</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                        |
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |

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