

# 21H,23H-Porphin,5,10,15,20-tetrakis(4-methylphen

|                             |                                                                                     |
|-----------------------------|-------------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C48H38N4/c1-29-5-13-33(14-6-29)45-37-21-23-39(49-37)46(34-15-7-30(2)8-1    |
| <b>InchiKey:</b>            | SFQNUQLWBBZIOZ-PJEPRTXSA-N                                                          |
| <b>Formula:</b>             | C48H38N4                                                                            |
| <b>SMILES:</b>              | Cc1ccc(-c2c3nc(c(-c4ccc(C)cc4)c4ccc([nH]4)c(-c4ccc(C)cc4)c4nc(c(-c5ccc(C)cc5)c5ccc2 |
| <b>Mol. weight [g/mol]:</b> | 670.84                                                                              |
| <b>CAS:</b>                 | 14527-51-6                                                                          |

## Physical Properties

| Property code | Value            | Unit   | Source         |
|---------------|------------------|--------|----------------|
| chs           | -24797.80 ± 8.10 | kJ/mol | NIST Webbook   |
| hfs           | 479.00 ± 10.00   | kJ/mol | NIST Webbook   |
| hsub          | 260.40           | kJ/mol | NIST Webbook   |
| log10ws       | -19.41           |        | Crippen Method |
| logp          | 11.593           |        | Crippen Method |
| mcvol         | 530.460          | ml/mol | McGowan Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C14527516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14527516&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |

## Legend

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <b>hfs:</b>     | Solid phase enthalpy of formation at standard conditions |
| <b>hsub:</b>    | Enthalpy of sublimation at standard conditions           |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l                       |
| <b>logp:</b>    | Octanol/Water partition coefficient                      |
| <b>mcvol:</b>   | McGowan's characteristic volume                          |

Latest version available from:

<https://www.cheméo.com/cid/17-158-8/21H-23H-Porphin-5-10-15-20-tetrakis-4-methylphenyl.pdf>

Generated by Cheméo on 2025-12-23 06:40:50.706291964 +0000 UTC m=+6220248.236332628.

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