# 2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphin

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|---|---|
| **Other names:** | Octaethylporphyrin |
| | 2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine |
| | Octaethylporphine |
| | 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octaethyl- |
| **Inchi:** | InChI=1S/C36H46N4/c1-9-21-22(10-2)30-18-32-25(13-5)26(14-6)34(39-32)20-36-28(16- |
| **InchiKey:** | HCIIFBHDBOCSAF-MUZKIALCSA-N |
| **Formula:** | C36H46N4 |
| **SMILES:** | CCC1=C(CC)c2cc3[nH]c(cc4nc(cc5[nH]c(cc1n2)c(CC)c5CC)C(CC)=C4CC)c(CC)c3CC |
| **Mol. weight [g/mol]:** | 534.78 |
| **CAS:** | 2683-82-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -20557.00 ± 21.00 | kJ/mol | NIST Webbook |
| ie | 6.39 ± 0.03 | eV | NIST Webbook |
| ie | 6.25 | eV | NIST Webbook |
| log10ws | -13.65 | | Crippen Method |
| logp | 9.062 | | Crippen Method |
| mcvol | 456.420 | ml/mol | McGowan Method |

## Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2683821&Units=SI |

## Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **ie:** | Ionization energy |

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

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