

Phthalocyanine

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| Other names: | 29H,31H-Phthalocyanine |
| Inchi: | InChI=1S/C32H18N8/c1-2-10-18-17(9-1)25-33-26(18)38-28-21-13-5-6-14-22(21)30(35-2 |
| InchiKey: | IEQIEDJGQAUEQZ-UHFFFAOYSA-N |
| Formula: | C32H18N8 |
| SMILES: | c1ccc2c(c1)-c1nc-2nc2[nH]c(nc3nc(nc4[nH]c(n1)c1cccc41)-c1cccc1-3)c1cccc21 |
| Mol. weight [g/mol]: | 514.54 |
| CAS: | 574-93-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| ie | 7.36 ± 0.10 | eV | NIST Webbook |
| log10ws | -14.96 | | Crippen Method |
| logp | 5.905 | | Crippen Method |
| mcpol | 362.140 | ml/mol | McGowan Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------------|--------|-----------------|--------------|
| hsubt | 223.80 ± 1.30 | kJ/mol | 648.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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=C574936&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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|-----------------|--|
| hsubt: | Enthalpy of sublimation at a given temperature |
| 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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