

# 21H,23H-Porphine-2,7,12,17-tetrapropanoic acid, 3,8,13,18-tetramethyl-, tetramethyl ester

Other names:

2,7,12,17-Porphinetetrapropionic acid, 3,8,13,18-tetramethyl-, tetramethyl ester  
Coproporphyrin I tetramethyl ester  
Coproporphyrin tetramethyl ester i  
Tetramethyl 3,8,13,18-tetramethyl-21H,23H-porphine-2,7,12,17-tetrapropionate

Inchi: InChI=1S/C40H46N4O8/c1-21-25(9-13-37(45)49-5)33-18-30-23(3)27(11-15-39(47)51-7)3

InchiKey: OVYASYKFNWTMII-QEMHYRKZSA-N

Formula: C40H46N4O8

SMILES: COC(=O)CCC1=C(C)c2cc3[nH]c(cc4nc(cc5[nH]c(cc1n2)c(C)c5CCC(=O)OC)C(C)=C4CC

Mol. weight [g/mol]: 710.82

CAS: 25767-20-8

## Physical Properties

| Property code | Value             | Unit   | Source         |
|---------------|-------------------|--------|----------------|
| chs           | -20834.00 ± 21.00 | kJ/mol | NIST Webbook   |
| log10ws       | -10.96            |        | Crippen Method |
| logp          | 5.947             |        | Crippen Method |
| mcvol         | 542.540           | 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](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=C25767208&Units=SI>

## Legend

chs: Standard solid enthalpy of combustion

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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