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

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