2,7,12,17-Tetraethyl-3,8,13,18-tetramethyl-21H,23H

Other names:	Etioporphyrin 21H,23H-Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- 3,8,13,18-Tetraethyl-2,7,12,17-tetramethyl-21H,23H-porphine Mesoetioporphyrin
Inchi:	InChI=1S/C32H38N4/c1-9-21-17(5)25-14-30-23(11-3)19(7)27(35-30)16-32-24(12-4)20(8)
InchiKey:	VIXIHEJFGRACDI-GCISPZHASA-N
Formula:	C32H38N4
SMILES:	CCC1=C(C)c2cc3[nH]c(cc4nc(cc5[nH]c(cc1n2)c(C)c5CC)C(C)=C4CC)c(C)c3CC
Mol. weight [g/mol]:	478.67
CAS:	448-71-5

Physical Properties

Property code	Value	Unit	Source
chs	-17998.00 ± 18.00	kJ/mol	NIST Webbook
ie	6.30	eV	NIST Webbook
log10ws	-12.16		Crippen Method
logp	7.774		Crippen Method
mcvol	400.060	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=C448715&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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