Mesoporphyrin ix dimethyl ester

Other names:	21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester Mesoporphyrin dimethyl ester 2,18-Porphinedipropionic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester Dimethyl 8,13-diethyl-3,7,12,17-tetramethyl-21H,23H-porphine-2,18-dipropionate dimethyl 7,12-diethyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropionate
Inchi:	InChI=1S/C36H42N4O4/c1-9-23-19(3)27-15-28-21(5)25(11-13-35(41)43-7)33(39-28)18-3
InchiKey:	LUUYUVIPWOKSNM-MFBGAUBSSA-N
Formula:	C36H42N4O4
SMILES:	CCC1=C(C)c2cc3[nH]c(cc4nc(cc5[nH]c(cc1n2)c(C)c5CCC(=O)OC)C(CCC(=O)OC)=C4C
Mol. weight [g/mol]:	594.74
CAS:	1263-63-4

Physical Properties

Property code	Value	Unit	Source
chs	-19345.00	kJ/mol	NIST Webbook
log10ws	-11.56		Crippen Method
logp	6.860		Crippen Method
mcvol	471.300	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1263634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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