Tetra(3-pyridyl)porphyrin

Inchi: InChI=1S/C40H26N8/c1-5-25(21-41-17-1)37-29-9-11-31(45-29)38(26-6-2-18-42-22-26)3
InchiKey: GZKPUYJFADMBGO-KHQKEXQOSA-N
Formula: C40H26N8
SMILES: C1=Cc2nc1c(-c1cccnc1)c1ccc([nH]1)c(-c1cccnc1)c1nc(c(-c3cccnc3)c3ccc([nH]3)c2-c2cc
Mol. weight [g/mol]: 618.69
CAS: 40882-83-5

Physical Properties

Property code	Value	Unit	Source
chs	-20268.00 ± 6.80	kJ/mol	NIST Webbook
hfs	811.80 ± 8.60	kJ/mol	NIST Webbook
hsub	270.40	kJ/mol	NIST Webbook
log10ws	-16.57		Crippen Method
logp	7.940		Crippen Method
mcvol	457.660	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=C40882835&Units=SI

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume