

Tetra(p-nitrophenyl)porphyrin

Inchi: InChI=1S/C44H26N8O8/c53-49(54)29-9-1-25(2-10-29)41-33-17-19-35(45-33)42(26-3-11
InchiKey: FVHZCBQLLFLQAG-LWQDQPMZSA-N
Formula: C44H26N8O8
SMILES: O=[N+]([O-])c1ccc(-c2c3nc(c(-c4ccc([N+](=O)[O-])cc4)c4ccc([nH]4)c(-c4ccc([N+](=O)[O-]
Mol. weight [g/mol]: 794.73
CAS: 22843-73-8

Physical Properties

Property code	Value	Unit	Source
chs	-21781.40 ± 9.50	kJ/mol	NIST Webbook
hfs	751.00 ± 11.00	kJ/mol	NIST Webbook
hsub	312.44	kJ/mol	NIST Webbook
log10ws	-20.11		Crippen Method
logp	9.993		Crippen Method
mcvol	543.780	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C22843738&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

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