

Tetraphenylporphyrin

Other names:	.alpha.,.beta.,.gamma.,.delta.-tetraphenylporphine 21H,23H-porphine, 5,10,15,20-tetraphenyl- 5,10,15,20-Tetraphenyl-21H,23H-porphyrin 5,10,15,20-tetraphenyl-21H,23H-porphine 5,10,15,20-tetraphenylporphine 5,10,15,20-tetraphenylporphyrin NSC 18506 NSC 640184 Tetraphenyl porphine meso-Tetraphenylporphyrine meso-tetraphenylporphine meso-tetraphenylporphyrin porphine, .alpha.,.beta.,.gamma.,.delta.-tetraphenyl- porphine, 5,10,15,20-tetraphenyl- tetraphenylporphine «alpha»,«beta»,«gamma»,«delta»-Tetraphenylporphine
Inchi:	InChI=1S/C44H30N4/c1-5-13-29(14-6-1)41-33-21-23-35(45-33)42(30-15-7-2-8-16-30)37-
InchiKey:	YNHJECZULSZAQK-LWQDQPMZSA-N
Formula:	C44H30N4
SMILES:	C1=Cc2nc1c(-c1cccc1)c1ccc([nH]1)c(-c1cccc1)c1nc(c(-c3cccc3)c3ccc([nH]3)c2-c2cc
Mol. weight [g/mol]:	614.74
CAS:	917-23-7

Physical Properties

Property code	Value	Unit	Source
chs	-22223.20 ± 6.30	kJ/mol	NIST Webbook
ea	1.69 ± 0.10	eV	NIST Webbook
hfs	621.30 ± 6.30	kJ/mol	NIST Webbook
hsub	244.20	kJ/mol	NIST Webbook
ie	6.39	eV	NIST Webbook
ie	6.30 ± 0.20	eV	NIST Webbook
log10ws	-17.50		Crippen Method
logp	10.360		Crippen Method
mcvol	474.100	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	142.00 ± 3.00	kJ/mol	666.50	NIST Webbook
hsubt	171.00 ± 2.00	kJ/mol	549.00	NIST Webbook
hsubt	110.90 ± 5.00	kJ/mol	633.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities and thermodynamics of TPP in propionic acid + water and	https://www.doi.org/10.1016/j.fluid.2015.03.039
Study of the stability of 5,10,15,20-tetraphenylporphine (TPP)	https://www.doi.org/10.1016/j.jct.2009.12.007
Solubilities of porphyrins NiTPP, CoTPP, CuTPP, and ZnTPP in benzene and	https://www.doi.org/10.1021/acs.jced.5b00092
5,10,15,20-tetraphenylporphine and	https://www.doi.org/10.1021/je501002a
5,10,15,20-tetraphenylporphine and	http://link.springer.com/article/10.1007/BF02311772
5,10,15,20-tetraphenylporphine and	http://webbook.nist.gov/cgi/cbook.cgi?ID=C917237&Units=SI
Manganese(III) Chloride in Binary	
Ethanol + Water Solvent Mixtures:	

Legend

chs:	Standard solid enthalpy of combustion
ea:	Electron affinity
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point

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