Tetra(p-bromophenyl)porphyrin

Inchi: InChI=1S/C44H26Br4N4/c45-29-9-1-25(2-10-29)41-33-17-19-35(49-33)42(26-3-11-30(46
InchiKey: ANWXWWSYNQLVED-LWQDQPMZSA-N
Formula: C44H26Br4N4
SMILES: Brc1ccc(-c2c3nc(c(-c4ccc(Br)cc4)c4ccc([nH]4)c(-c4ccc(Br)cc4)c4nc(c(-c5ccc(Br)cc5)c5c
Mol. weight [g/mol]: 930.32
CAS: 29162-73-0

Physical Properties

Property code	Value	Unit	Source
chs	-21784.00 ± 11.00	kJ/mol	NIST Webbook
hfs	754.00 ± 13.00	kJ/mol	NIST Webbook
hsub	284.00	kJ/mol	NIST Webbook
log10ws	-22.15		Crippen Method
logp	13.410		Crippen Method
mcvol	544.100	ml/mol	McGowan Method

Sources

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=C29162730&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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