Hexadecabromophthalocyanine

Inchi: InChI=1S/C32H2Br16N8/c33-9-1-2(10(34)18(42)17(9)41)26-49-25(1)53-27-3-4(12(36)20
InchiKey: UJMYDIWJKAQQMT-UHFFFAOYSA-N
Formula: C32H2Br16N8
SMILES: Brc1c(Br)c(Br)c2c(c1Br)-c1nc-2nc2[nH]c(nc3nc(nc4[nH]c(n1)c1c(Br)c(Br)c(Br)c(Br)c41)-c
Mol. weight [g/mol]: 1776.88
CAS: 28746-04-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-33.57		Crippen Method
logp	18.105		Crippen Method
mcvol	642.140	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	109.00 ± 16.00	kJ/mol	465.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28746045&Units=SI
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

Legend

hsubt: Enthalpy of sublimation at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume