

# 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/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

Latest version available from:

<https://www.cheméo.com/cid/59-927-8/Hexadecabromophthalocyanine.pdf>

Generated by Cheméo on 2024-04-20 06:55:43.551678939 +0000 UTC m=+15885392.472256253.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.