

Tribenzo[a,e,i]cyclododecene,5,6,11,12,17,18-hexa

Inchi: InChI=1S/C24H12/c1-2-8-20-15-16-22-10-5-6-12-24(22)18-17-23-11-4-3-9-21(23)14-13-
InchiKey: FYTAWGCRZIWNNOV-UHFFFAOYSA-N
Formula: C24H12
SMILES: C1#Cc2ccccc2C#Cc2ccccc2C#Cc2ccccc21
Mol. weight [g/mol]: 300.35
CAS: 5385-26-2

Physical Properties

Property code	Value	Unit	Source
ie	7.45	eV	NIST Webbook
log10ws	-6.96		Crippen Method
logp	4.199		Crippen Method
mcvol	241.080	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=C5385262&Units=SI>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/72-406-1/Tribenzo-a-e-i-cyclododecene-5-6-11-12-17-18-hexadehydro.pdf>

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