

# Dibenzo[a,e]cyclooctene,5,6,11,12-tetrahydro-

**Inchi:** InChI=1S/C16H8/c1-2-6-14-11-12-16-8-4-3-7-15(16)10-9-13(14)5-1/h1-8H  
**InchiKey:** JFYLRMKUYCIWMX-UHFFFAOYSA-N  
**Formula:** C16H8  
**SMILES:** C1#Cc2ccccc2C#Cc2ccccc21  
**Mol. weight [g/mol]:** 200.23  
**CAS:** 53397-65-2

## Physical Properties

Property code	Value	Unit	Source
ie	7.76	eV	NIST Webbook
log10ws	-4.55		Crippen Method
logp	2.800		Crippen Method
mcvol	160.720	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53397652&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## 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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