

Dibenzo[a,e]cyclooctene,5,6-didehydro-

Inchi:	InChI=1S/C16H10/c1-2-6-14-11-12-16-8-4-3-7-15(16)10-9-13(14)5-1/h1-10H
InchiKey:	GVOYLOQRZIUYYOL-UHFFFAOYSA-N
Formula:	C16H10
SMILES:	C1#Cc2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]:	202.25
CAS:	53397-66-3

Physical Properties

Property code	Value	Unit	Source
ie	7.56	eV	NIST Webbook
log10ws	-4.74		Crippen Method
logp	3.570		Crippen Method
mcvol	165.020	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=C53397663&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/73-986-7/Dibenzo-a-e-cyclooctene-5-6-didehydro.pdf>

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