Dibenzo[a,c]cyclododecene, 5,6,11,12-tetradehydro-7,8,9,10-tetrahydro-

Inchi: InChI=1S/C20H16/c1-2-4-6-12-18-14-8-10-16-20(18)19-15-9-7-13-17(19)11-5-3-1/h7-10,

InchiKey: TVOBLVHRGDRRBQ-UHFFFAOYSA-N

Formula: C20H16

SMILES: C1#Cc2ccccc2-c2ccccc2C#CCCCC1

Mol. weight [g/mol]: 256.34

CAS: 36398-39-7

Physical Properties

Property code	Value	Unit	Source
ie	7.90	eV	NIST Webbook
ie	8.04	eV	NIST Webbook
log10ws	-7.04		Crippen Method
logp	4.631		Crippen Method
mcvol	217.080	ml/mol	McGowan Method

Sources

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=C36398397&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume