7H-Dibenzo-8,9,10,11-tetrahydro-

Inchi: InChI=1S/C21H18/c1-2-4-6-12-18-14-8-10-16-20(18)21-17-11-9-15-19(21)13-7-5-3-1/h8-
InchiKey: ZXDRPLPGXKZLMT-UHFFFAOYSA-N
Formula: C21H18
SMILES: C1#Cc2ccccc2-c2ccccc2C#CCCCCC1
Mol. weight [g/mol]: 270.37
CAS: 78631-72-8

Physical Properties

Property code	Value	Unit	Source
ie	7.70	eV	NIST Webbook
ie	8.04	eV	NIST Webbook
log10ws	-7.46		Crippen Method
logp	5.021		Crippen Method
mcvol	231.170	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C78631728&Units=SI

Legend

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