

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/h8-11
InchiKey: ZXDRPLPGXKZLMT-UHFFFAOYSA-N
Formula: C21H18
SMILES: C1#Cc2ccccc2-c2ccccc2C#CCCCC1
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/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=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

Latest version available from:

<https://www.chemeo.com/cid/30-174-5/7H-Dibenzo-8-9-10-11-tetrahydro.pdf>

Generated by Cheméo on 2024-04-27 23:19:52.823397686 +0000 UTC m=+16549241.743974997.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.