5H-Dibenz[c,e]azepine, 6,7-dihydro-6-(2-propenyl)-

Other names: 5H-Dibenz(c,e)azepine, 6-allyl-6,7-dihydro-
6-Allil-6,7-diidro-5H-dibenzo(c,l)azepina
6-Allyl-6,7-dihydro-5H-dibenz(c,e)azepine
Azapetina
Azapetine
5H-Dibenz(c,e)azepine, 6,7-dihydro-6-allyl-
Ilidar base
1-Allyl-2,7-dihydro-3,4:5,6-dibenzazepine

Inchi: InChI=1S/C17H17N/c1-2-11-18-12-14-7-3-5-9-16(14)17-10-6-4-8-15(17)13-18/h2-10H,1,

InchiKey: NYGHGTMKALXFIA-UHFFFAOYSA-N

Formula: C17H17N

SMILES: C=CCN1Cc2ccccc2-c2ccccc2C1

Mol. weight [g/mol]: 235.32

CAS: 146-36-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	3.855		Crippen Method
mcvol	197.690	ml/mol	McGowan Method
rinpol	1917.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1939.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C146361&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices