

2-Azahexahelicene

Inchi: InChI=1S/C25H15N/c1-2-4-17-8-20-11-23-13-24-14-25-15-26-6-5-18(25)9-21(24)12-22(24)3
InchiKey: FNJOTLVUHMJBQG-UHFFFAOYSA-N
Formula: C25H15N
SMILES: c1ccc2cc3cc4cc5cc6cnccc6cc5cc4cc3cc2c1
Mol. weight [g/mol]: 329.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.26		Crippen Method
logp	6.848		Crippen Method
mcvol	252.030	ml/mol	McGowan Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525298&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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