

2-Azaoctahelicene

Inchi: InChI=1S/C33H19N/c1-2-4-21-8-24-11-27-14-30-16-31-17-32-18-33-19-34-6-5-22(33)9-2
InchiKey: UJCSRZDEPGLBFD-UHFFFAOYSA-N
Formula: C33H19N
SMILES: c1ccc2cc3cc4cc5cc6cc7cc8cnccc8cc7cc6cc5cc4cc3cc2c1
Mol. weight [g/mol]: 429.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.87		Crippen Method
logp	9.154		Crippen Method
mcvol	325.830	ml/mol	McGowan Method
rinpol	3873.00		NIST Webbook
rinpol	3873.00		NIST Webbook

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=R525307&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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