2-Azaheptahelicene

Inchi: InChI=1S/C29H17N/c1-2-4-19-8-22-11-25-14-27-15-28-16-29-17-30-6-5-20(29)9-23(28)1
InchiKey: ZUXGJDCRCLNDCD-UHFFFAOYSA-N
Formula: C29H17N
SMILES: c1ccc2cc3cc4cc5cc6cc7cnccc7cc6cc5cc4cc3cc2c1
Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.06		Crippen Method
logp	8.001		Crippen Method
mcvol	288.930	ml/mol	McGowan Method
rinpol	3577.00		NIST Webbook
rinpol	3577.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525283&Units=SI
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

Legend

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

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