

2-Azafluoranthene

Inchi: InChI=1S/C15H9N/c1-2-6-12-11(5-1)13-7-3-4-10-8-16-9-14(12)15(10)13/h1-9H
InchiKey: AZEXTOPKZARAGZ-UHFFFAOYSA-N
Formula: C15H9N
SMILES: c1ccc2c(c1)-c1cccc3cncc-2c13
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	3.882		Crippen Method
mcvol	154.350	ml/mol	McGowan Method
rinpol	347.15		NIST Webbook
rinpol	346.74		NIST Webbook
rinpol	347.39		NIST Webbook
rinpol	347.39		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R53717&Units=SI>

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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