4-Azachrysene

Inchi: InChI=1S/C17H11N/c1-2-4-14-12(3-1)5-8-16-15(14)7-6-13-9-10-18-11-17(13)16/h1-11H
InchiKey: XLASABQETKYXNT-UHFFFAOYSA-N
Formula: C17H11N
SMILES: c1ccc2c(c1)ccc1c3cnccc3ccc21
Mol. weight [g/mol]: 229.28
CAS: 218-19-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	4.541		Crippen Method
mcvol	178.230	ml/mol	McGowan Method
rinpol	401.43		NIST Webbook
rinpol	401.16		NIST Webbook
rinpol	401.16		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=C218199&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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