

# 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](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/ci9903071>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/28-073-0/4-Azachrysene.pdf>

Generated by Cheméo on 2024-04-29 04:28:57.336862386 +0000 UTC m=+16654186.257439698.

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