

# 1H-Benz[fg]aceanthrylene

|                             |                                                                                   |
|-----------------------------|-----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C19H12/c1-2-6-15-14(5-1)16-7-3-4-12-8-9-13-10-11-17(15)19(13)18(12)16/h1 |
| <b>InchiKey:</b>            | CBTNLQKGXWTRFH-UHFFFAOYSA-N                                                       |
| <b>Formula:</b>             | C19H12                                                                            |
| <b>SMILES:</b>              | <chem>C1=c2ccc3cccc4c5ccccc5c(c2c34)C1</chem>                                     |
| <b>Mol. weight [g/mol]:</b> | 240.30                                                                            |
| <b>CAS:</b>                 | 193-69-1                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.60   |        | Crippen Method |
| logp          | 4.202   |        | Crippen Method |
| mcvol         | 185.570 | ml/mol | McGowan Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C193691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C193691&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |

Latest version available from:

<https://www.chemeo.com/cid/78-324-6/1H-Benz-fg-aceanthrylene.pdf>

Generated by Cheméo on 2025-12-07 05:51:10.618322129 +0000 UTC m=+4834868.148362784.

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