

Indeno[2,1-a]phenalene

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C20H12/c1-2-9-16-14(5-1)11-19-17-10-4-7-13-6-3-8-15(20(13)17)12-18(16)19 |
| InchiKey: | CGNGNSAJKKWGNN-UHFFFAOYSA-N |
| Formula: | C20H12 |
| SMILES: | C1=c2c(cc3cccc4cccc2c43)-c2cccc21 |
| Mol. weight [g/mol]: | 252.31 |
| CAS: | 200-71-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.08 | | Crippen Method |
| logp | 4.521 | | Crippen Method |
| mcvol | 195.360 | ml/mol | McGowan Method |

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=C200715&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 |

Latest version available from:

<https://www.chemeo.com/cid/75-868-6/Indeno-2-1-a-phenalene.pdf>

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