

2-Benzylquinoline

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C16H13N/c1-2-6-13(7-3-1)12-15-11-10-14-8-4-5-9-16(14)17-15/h1-11H,12H2 |
| InchiKey: | LLVHFJHCODIQJH-UHFFFAOYSA-N |
| Formula: | C16H13N |
| SMILES: | <chem>c1ccc(Cc2ccc3ccccc3n2)cc1</chem> |
| Mol. weight [g/mol]: | 219.28 |
| CAS: | 1745-77-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.14 | | Crippen Method |
| logp | 3.826 | | Crippen Method |
| mcpvol | 179.300 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 420.50 ± 2.50 | K | 0.01 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1745773&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

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