

# 2-Pyridinamine, N-(phenylmethyl)-

|                      |                                                                                                                          |
|----------------------|--------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Pyridine, 2-(benzylamino)-<br>2-(Benzylamino)pyridine<br>N-benzylpyridin-2-amine<br>Tripelenamine M (Benzylpyridylamine) |
| Inchi:               | InChI=1S/C12H12N2/c1-2-6-11(7-3-1)10-14-12-8-4-5-9-13-12/h1-9H,10H2,(H,13,14)                                            |
| InchiKey:            | WYHXNQXDQQMTQI-UHFFFAOYSA-N                                                                                              |
| Formula:             | C12H12N2                                                                                                                 |
| SMILES:              | c1ccc(CNc2ccccc2)cc1                                                                                                     |
| Mol. weight [g/mol]: | 184.24                                                                                                                   |
| CAS:                 | 6935-27-9                                                                                                                |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.36   |        | Crippen Method |
| logp          | 2.694   |        | Crippen Method |
| mcvol         | 152.380 | ml/mol | McGowan Method |
| rinpol        | 1650.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6935279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6935279&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |

## 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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<https://www.chemeo.com/cid/94-165-5/2-Pyridinamine-N-phenylmethyl.pdf>

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