

7H-tetrazolo[5,1-i]purine, 7-benzyl-

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H9N7/c1-2-4-9(5-3-1)6-18-7-13-10-11(18)14-8-19-12(10)15-16-17-19/h1-5 |
| InchiKey: | HOHUVIRJDOLSQB-UHFFFAOYSA-N |
| Formula: | C12H9N7 |
| SMILES: | <chem>c1ccc(Cn2cnc3c2ncn2nnnc32)cc1</chem> |
| Mol. weight [g/mol]: | 251.25 |
| CAS: | 10553-44-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.62 | | Crippen Method |
| logp | 0.917 | | Crippen Method |
| mcvol | 171.960 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C10553443&Units=SI |

Legend

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

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