

4-amino-1-[4-fluoro-5-(hydroxymethyl)oxolan-2-yl]

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|-----------------------------|---|
| Inchi: | InChI=1S/C9H12FN3O3/c10-5-3-8(16-6(5)4-14)13-2-1-7(11)12-9(13)15/h1-2,5-6,8,14H,3 |
| InchiKey: | HNSUDSIHCJEYQG-UHFFFAOYSA-N |
| Formula: | C9H12FN3O3 |
| SMILES: | Nc1ccn(C2CC(F)C(CO)O2)c(=O)n1 |
| Mol. weight [g/mol]: | 229.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| log10ws | -1.18 | | Aqueous Solubility Prediction Method |
| logp | -0.557 | | Crippen Method |
| mcvol | 152.370 | ml/mol | McGowan Method |

Sources

| | |
|--|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Aqueous Solubility Prediction Method: | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |

Legend

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

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