

2-Amino-4,6-dihydroxypyrimidine, N,O,O'-tris(pentafluoropropionyl)-

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C13H2F15N3O5/c14-8(15,11(20,21)22)4(32)31-7-29-2(35-5(33)9(16,17)12(23 |
| InchiKey: | ZAIGGKWWEMSTJZ-UHFFFAOYSA-N |
| Formula: | C13H2F15N3O5 |
| SMILES: | O=C(Nc1nc(OC(=O)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)F)n1)C(F)(F)C(F)(F)F |
| Mol. weight [g/mol]: | 565.15 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.02 | | Crippen Method |
| logp | 3.819 | | Crippen Method |
| mcvol | 243.210 | ml/mol | McGowan Method |
| rinpol | 1215.00 | | NIST Webbook |

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=U375760&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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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