

5-Hydroxyindole, N,O-bis(trifluoroacetyl)-

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H5F6NO3/c13-11(14,15)9(20)19-4-3-6-5-7(1-2-8(6)19)22-10(21)12(16,17) |
| InchiKey: | GGMVDPJXIJBSFF-UHFFFAOYSA-N |
| Formula: | C12H5F6NO3 |
| SMILES: | O=C(Oc1ccc2c(ccn2C(=O)C(F)(F)F)c1)C(F)(F)F |
| Mol. weight [g/mol]: | 325.16 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.03 | | Crippen Method |
| logp | 3.312 | | Crippen Method |
| mcvol | 170.630 | ml/mol | McGowan Method |
| rinpola | 1963.00 | | 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=U375683&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

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

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