# 4'-hydroxy-1-(3-trifluoromethylphenyl)piperazine, diTFA

| | |
|---|---|
| **InChi:** | InChI=1S/C15H11F9N2O3/c16-13(17,18)9-7-8(1-2-10(9)29-12(28)15(22,23)24)25-3-5-26 |
| **InchiKey:** | FRQQAVKJHQNQJP-UHFFFAOYSA-N |
| **Formula:** | C15H11F9N2O3 |
| **SMILES:** | O=C(Oc1ccc(N2CCN(C(=O)C(F)(F)F)CC2)cc1C(F)(F)F)C(F)(F)F |
| **Mol. weight [g/mol]:** | 438.25 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.04 | | Crippen Method |
| logp | 3.384 | | Crippen Method |
| mcvol | 232.490 | ml/mol | McGowan Method |
| rinpol | 1783.00 | | NIST Webbook |
| rinpol | 1783.00 | | NIST Webbook |

## Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R418690&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

## Legend

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|---|---|
| **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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