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

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=R418690&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

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.