

Tyramine N-TFA-O-TMS

Inchi: InChI=1S/C13H18F3NO3Si/c1-21(2,3)20-11-6-4-10(5-7-11)8-9-17-19-12(18)13(14,15)16
InchiKey: FZXKDJBCTDJZSC-UHFFFAOYSA-N
Formula: C13H18F3NO3Si
SMILES: C[Si](C)(C)Oc1ccc(CCNO(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 321.37

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.82 | | Crippen Method |
| logp | 3.053 | | Crippen Method |
| rinpol | 1621.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R83827&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/37-395-3/Tyramine-N-TFA-O-TMS.pdf>

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