

Hippuric acid, 3-hydroxy, TMS, # 1

Inchi: InChI=1S/C18H33NO4Si3/c1-24(2,3)21-16-12-10-11-15(13-16)18(23-26(7,8)9)19-14-17(20)
InchiKey: DMQDEQYREHGSLU-HNENSFHCSA-N
Formula: C18H33NO4Si3
SMILES: C[Si](C)(C)OC(=O)CN=C(O[Si](C)(C)C)c1cccc(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 411.72

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.97 | | Crippen Method |
| logp | 4.877 | | Crippen Method |
| rinpol | 2055.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94674&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/68-671-2/Hippuric-acid-3-hydroxy-TMS-1.pdf>

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