

Hippuric acid, 4-amino, TMS, # 1

Inchi: InChI=1S/C18H34N2O3Si3/c1-24(2,3)20-16-12-10-15(11-13-16)18(23-26(7,8)9)19-14-17
InchiKey: PWLOKNZTDWKGGG-HNENSFHCSA-N
Formula: C18H34N2O3Si3
SMILES: C[Si](C)(C)Nc1ccc(C(=NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 410.73

Physical Properties

Property code	Value	Unit	Source
log10ws	2.09		Crippen Method
logp	4.910		Crippen Method
rinpol	2300.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94692&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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