

2-Hydroxyhippuric acid, tert-butyl dimethylsilyl ether, tert-butyl dimethylsilyl ester

Other names:

2-Hydroxyhippuric acid, TBDMS

Inchi: InChI=1S/C21H37NO4Si2/c1-20(2,3)27(7,8)25-17-14-12-11-13-16(17)19(24)22-15-18(23)

InchiKey: XLUDASZJNZYLKY-UHFFFAOYSA-N

Formula: C₂₁H₃₇NO₄Si₂

SMILES: CC(C)(C)[Si](C)(C)OC(=O)CNC(=O)c1ccccc1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 423.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	5.349		Crippen Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U364433&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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