

Salicyluric acid, tris(trimethylsilyl)- deriv.

Other names:	Hippuric acid, 2-hydroxy, TMS, #1
Inchi:	InChI=1S/C18H33NO4Si3/c1-24(2,3)21-16-13-11-10-12-15(16)18(23-26(7,8)9)19-14-17(
InchiKey:	JBFNXVAKDSIUSE-UHFFFAOYSA-N
Formula:	C18H33NO4Si3
SMILES:	C[Si](C)(C)OC(=O)CN=C(O[Si](C)(C)C)c1ccccc1O[Si](C)(C)C
Mol. weight [g/mol]:	411.72

Physical Properties

Property code	Value	Unit	Source
log10ws	1.97		Crippen Method
logp	4.877		Crippen Method
rinsol	1954.00		NIST Webbook
rinsol	1909.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U79279&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/12-544-4/Salicyluric-acid-tris-trimethylsilyl-deriv.pdf>

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