

3-Hydroxyhippuric acid, di-TMS

Other names:	Hippuric acid, 3-hydroxy, TMS, #2
Inchi:	InChI=1S/C15H25NO4Si2/c1-21(2,3)19-13-9-7-8-12(10-13)15(18)16-11-14(17)20-22(4,5)
InchiKey:	VBPOBZKSUYGRGI-UHFFFAOYSA-N
Formula:	C15H25NO4Si2
SMILES:	C[Si](C)(C)OC(=O)CNC(=O)c1cccc(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	339.53
CAS:	56272-74-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.59		Crippen Method
logp	3.008		Crippen Method
rinpol	2117.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2121.00		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=C56272743&Units=SI

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/32-909-7/3-Hydroxyhippuric-acid-di-TMS.pdf>

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