

Hippuric acid, bis-TMS

Other names:	Hippuric acid (benzoylglycine), bis-TMS Hyp, TMS Hippuric acid, TMS, # 1
Inchi:	InChI=1S/C15H25NO3Si2/c1-20(2,3)18-14(17)12-16-15(19-21(4,5)6)13-10-8-7-9-11-13/h1-13,15-17,20-21
InchiKey:	XPDMZDVUZMUQAX-NXVVXOECSA-N
Formula:	C15H25NO3Si2
SMILES:	C[Si](C)(C)OC(=O)CN=C(O[Si](C)(C)C)c1ccccc1
Mol. weight [g/mol]:	323.53

Physical Properties

Property code	Value	Unit	Source
log10ws	0.98		Crippen Method
logp	3.663		Crippen Method
rinpol	1785.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1792.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R7804&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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