

6-Hydroxynicotinic acid di-tms derivative

Other names:	6-Hydroxynicotinic acid, trimethylsilyl ether, trimethylsilyl ester Trimethylsilyl 6-[(trimethylsilyl)oxy]nicotinate 6-Hydroxynicotinic acid, 2tms derivative
Inchi:	InChI=1S/C12H21NO3Si2/c1-17(2,3)15-11-8-7-10(9-13-11)12(14)16-18(4,5)6/h7-9H,1-6H
InchiKey:	PKMMPWFEAYNEKL-UHFFFAOYSA-N
Formula:	C12H21NO3Si2
SMILES:	C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)nc1
Mol. weight [g/mol]:	283.48

Physical Properties

Property code	Value	Unit	Source
logp	3.287		Crippen Method
rinpol	1569.90		NIST Webbook
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Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C36972824&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/120-488-7/6-Hydroxynicotinic-acid-di-tms-derivative.pdf>

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