

3-Pyridinecarboxylic acid, 6-[(trimethylsilyl)oxy]-, trimethylsilyl ester

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,1-6

InchiKey: PKMMPWFEAYNEKL-UHFFFAOYSA-N

Formula: C₁₂H₂₁NO₃Si₂

SMILES: C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)nc1

Mol. weight [g/mol]: 283.47

CAS: 36972-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.62		Crippen Method
logp	3.287		Crippen Method
rinpol	1569.90		NIST Webbook
rinpol	1569.90		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=C36972824&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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