

# Nicotinamide, TMS

**Inchi:** InChI=1S/C12H22N2OSi2/c1-16(2,3)14-12(15-17(4,5)6)11-8-7-9-13-10-11/h7-10H,1-6H3  
**InchiKey:** APOOWQWYEKRGKA-WYMLVPIESA-N  
**Formula:** C12H22N2OSi2  
**SMILES:** C[Si](C)(C)N=C(O[Si](C)(C)C)c1cccnc1  
**Mol. weight [g/mol]:** 266.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.92		Crippen Method
logp	3.515		Crippen Method
rinpol	1458.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1458.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R5284&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/26-564-7/Nicotinamide-TMS.pdf>

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