

Niacinamide, N-trimethylsilyl-

Inchi:	InChI=1S/C9H14N2OSi/c1-13(2,3)11-9(12)8-5-4-6-10-7-8/h4-7H,1-3H3,(H,11,12)
InchiKey:	VQRBOHGTTOAYTJ-UHFFFAOYSA-N
Formula:	C9H14N2OSi
SMILES:	C[Si](C)(C)NC(=O)c1cccnc1
Mol. weight [g/mol]:	194.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.47		Crippen Method
logp	1.646		Crippen Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/64-009-1/Niacinamide-N-trimethylsilyl.pdf>

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