Niacinamide, N-tert.-butyldimethylsilyl-

Inchi: InChI=1S/C12H20N2OSi/c1-12(2,3)16(4,5)14-11(15)10-7-6-8-13-9-10/h6-9H,1-5H3,(H,14
InchiKey: WYKVTPXLQWXFSC-UHFFFAOYSA-N
Formula: C12H20N2OSi
SMILES: CC(C)(C)[Si](C)(C)N=C(O)c1cccnc1
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.27		Crippen Method
logp	3.391		Crippen Method
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374744&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/85-159-2/Niacinamide-N-tert-butyldimethylsilyl.pdf
Generated by Cheméo on 2024-10-12 03:50:51.387217652 +0000 UTC m=+3285914.024186901.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.