

(R,S)-Norcotinine, trimethylsilyl derivative

Inchi: InChI=1S/C12H18N2OSi/c1-16(2,3)14-11(6-7-12(14)15)10-5-4-8-13-9-10/h4-5,8-9,11H,6
InchiKey: MJNKENRJCHNGTP-UHFFFAOYSA-N
Formula: C12H18N2OSi
SMILES: C[Si](C)(C)N1C(=O)CCC1c1cccnc1
Mol. weight [g/mol]: 234.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	2.580		Crippen Method
rinpol	1735.80		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417213&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/114-589-2/R-S-Norcotinine-trimethylsilyl-derivative.pdf>

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