Quinaldinic acid, TMS

Inchi: InChI=1S/C13H15NO2Si/c1-17(2,3)16-13(15)12-9-8-10-6-4-5-7-11(10)14-12/h4-9H,1-3H
InchiKey: OWKSMABGDRGKBJ-UHFFFAOYSA-N
Formula: C13H15NO2Si
SMILES: C[Si](C)(C)OC(=O)c1ccc2ccccc2n1
Mol. weight [g/mol]: 245.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	3.226		Crippen Method
rinpol	1757.00		NIST Webbook
rinpol	1757.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R95359&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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