

Quinolinic acid, bis(trimethylsilyl) ester

Other names: Quinolinic acid, bis-TMS
Quinolinic acid, TMS
Quinolinic acid, 2tms derivative

Inchi: InChI=1S/C13H21NO4Si2/c1-19(2,3)17-12(15)10-8-7-9-14-11(10)13(16)18-20(4,5)6/h7-9

InchiKey: FUIIPFHUXKUVDX-UHFFFAOYSA-N

Formula: C13H21NO4Si2

SMILES: C[Si](C)(C)OC(=O)c1cccnc1C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 311.48

Physical Properties

Property code	Value	Unit	Source
log10ws	0.50		Crippen Method
logp	3.065		Crippen Method
rinpol	1745.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1745.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U143088&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/22-339-1/Quinolinic-acid-bis-trimethylsilyl-ester.pdf>

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