

3-Indoleacrylic acid, N-(tert-butyldimethylsilyl)-, (tert-butyldimethylsilyl) ester

Other names:

3-Indoleacrylic acid, tert-butyls derivative

InChI: InChI=1S/C23H37NO2Si2/c1-22(2,3)27(7,8)24-17-18(19-13-11-12-14-20(19)24)15-16-21

InchiKey: ZSWUJZBMQJQDEU-FOCLMDBBSA-N

Formula: C23H37NO2Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)C=Cc1cn([Si](C)(C)C(C)(C)C)c2ccccc12

Mol. weight [g/mol]: 415.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	7.056		Crippen Method
rinpol	1953.70		NIST Webbook
rinpol	1953.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333119&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/118-353-9/3-Indoleacrylic-acid-N-tert-butyldimethylsilyl-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-28 18:37:13.29664984 +0000 UTC m=+16618682.217227152.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.