

tert-Butyldimethylsilyl 2-[(3,5,6-trichloro-2-pyridyl)oxy]acetate

Other names: 2-[(3,5,6-Trichloro-2-pyridyl)oxy]acetic acid, tert-butyldimethylsilyl ester

Inchi: InChI=1S/C13H18Cl3NO3Si/c1-13(2,3)21(4,5)20-10(18)7-19-12-9(15)6-8(14)11(16)17-12

InchiKey: NMGZSKGQOGLATJ-UHFFFAOYSA-N

Formula: C13H18Cl3NO3Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)COc1nc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 370.73

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.26 | | Crippen Method |
| logp | 4.969 | | Crippen Method |
| rinpol | 2054.00 | | NIST Webbook |

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373119&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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