

# 5-Chloro-1-trimethylsilyl-indole-2-carboxylic acid, trimethylsilyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 5-Chloro-1H-indole-2-carboxylic acid, N,O-diTMS                                   |
| <b>Inchi:</b>               | InChI=1S/C15H22ClNO2Si2/c1-20(2,3)17-13-8-7-12(16)9-11(13)10-14(17)15(18)19-21(4) |
| <b>InchiKey:</b>            | ALKZKHLLNOLNC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C15H22ClNO2Si2  |
| <b>SMILES:</b>              | C[Si](C)(C)OC(=O)c1cc2cc(Cl)ccc2n1[Si](C)(C)C                                     |
| <b>Mol. weight [g/mol]:</b> | 339.96  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.43   |      | Crippen Method |
| logp          | 4.969   |      | Crippen Method |
| rinpol        | 2088.00 |      | NIST Webbook   |
| rinpol        | 2088.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373122&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>rinpol:</b>  | Non-polar retention indices         |

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