

# TMS

## 1-TMS-5-TMSOXY-3-(2-TMSAMINO)INDOLEPROPIONATE

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | TMS 1-TMS-5-TMSoxy-3-(2-TMSamino)indolepropionate<br>5-OH-Try, TMS               |
| Inchi:               | InChI=1S/C23H44N2O3Si4/c1-29(2,3)24-21(23(26)28-32(10,11)12)15-18-17-25(30(4,5)6 |
| InchiKey:            | OPTSZAFVDMCAQY-UHFFFAOYSA-N                                                      |
| Formula:             | C23H44N2O3Si4                                                                    |
| SMILES:              | C[Si](C)(C)NC(Cc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12)C(=O)O[Si](C)(C)C        |
| Mol. weight [g/mol]: | 508.96                                                                           |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| logp          | 6.252   |      | Crippen Method |
| rinpol        | 2460.00 |      | NIST Webbook   |
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## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method:           | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C69937479&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C69937479&amp;Units=SI</a> |

## Legend

|         |                                     |
|---------|-------------------------------------|
| logp:   | Octanol/Water partition coefficient |
| rinpol: | Non-polar retention indices         |

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