

TIGLYLGLYCINE diTMS

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|-----------------------------|---|
| Other names: | Tiglylglycine, bis-TMS |
| Inchi: | InChI=1S/C13H27NO3Si2/c1-9-11(2)13(17-19(6,7)8)14-10-12(15)16-18(3,4)5/h9H,10H2 |
| InchiKey: | CKXCZPIUSXILOC-FGWKFWITSA-N |
| Formula: | C13H27NO3Si2 |
| SMILES: | CC=C(C)C(=NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C |
| Mol. weight [g/mol]: | 301.53 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.17 | | Crippen Method |
| logp | 3.581 | | Crippen Method |
| rinpola | 1550.00 | | NIST Webbook |
| rinpola | 1564.00 | | NIST Webbook |
| rinpola | 1599.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R273531&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/14-029-4/TIGLYLGLYCINE-diTMS.pdf>

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