

3-Methyladipic acid, TBDMS

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| Other names: | 3-Methyladipic acid, DMTBS 3-Methyladipic acid, diTBDMS |
| Inchi: | InChI=1S/C19H40O4Si2/c1-15(14-17(21)23-25(10,11)19(5,6)7)12-13-16(20)22-24(8,9)18 |
| InchiKey: | OODFVLTWVRCTLQ-UHFFFAOYSA-N |
| Formula: | C19H40O4Si2 |
| SMILES: | CC(CCC(=O)O[Si](C)(C)C(C)(C)C)CC(=O)O[Si](C)(C)C(C)(C)C |
| Mol. weight [g/mol]: | 388.69 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.36 | | Crippen Method |
| logp | 5.890 | | Crippen Method |
| rinpol | 1990.00 | | NIST Webbook |
| rinpol | 1988.43 | | NIST Webbook |
| rinpol | 1991.00 | | NIST Webbook |
| rinpol | 1973.00 | | NIST Webbook |
| rinpol | 1989.00 | | NIST Webbook |
| rinpol | 1990.00 | | NIST Webbook |
| rinpol | 1989.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U221775&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

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