

Succinylacetone, TBDMS # 3

Inchi: InChI=1S/C19H38O4Si2/c1-15(20)14-16(22-24(8,9)18(2,3)4)12-13-17(21)23-25(10,11)19
InchiKey: AFAGHMMNXDARQM-UHFFFAOYSA-N
Formula: C19H38O4Si2
SMILES: CC(=O)CC(=CCC(=O)O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 386.67

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.46 | | Crippen Method |
| logp | 5.810 | | Crippen Method |
| rinpol | 1817.00 | | NIST Webbook |
| rinpol | 1825.00 | | NIST Webbook |
| rinpol | 1817.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R565023&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/59-073-6/Succinylacetone-TBDMS-3.pdf>

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