

3-Ketobutyric acid, oxime, di-TMS, #1

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|-----------------------------|---|
| Inchi: | InChI=1S/C10H23NO3Si2/c1-9(11-14-16(5,6)7)8-10(12)13-15(2,3)4/h8H2,1-7H3/b11-9+ |
| InchiKey: | TZPNNUWYLUYPBF-PKNCBQFBNSA-N |
| Formula: | C10H23NO3Si2 |
| SMILES: | CC(CC(=O)O[Si](C)(C)C)=NO[Si](C)(C)C |
| Mol. weight [g/mol]: | 261.47 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.79 | | Crippen Method |
| logp | 2.982 | | Crippen Method |
| rinpol | 1244.00 | | NIST Webbook |
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| rinpol | 1244.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R51585&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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.chemeo.com/cid/115-463-0/3-Ketobutyric-acid-oxime-di-TMS-1.pdf>

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