

# Cyclohexanecarboxylic acid, DMTBS

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C13H26O2Si/c1-13(2,3)16(4,5)15-12(14)11-9-7-6-8-10-11/h11H,6-10H2,1-5H3 |
| <b>InchiKey:</b>            | CQDVUROWLWGDJQ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C13H26O2Si   |
| <b>SMILES:</b>              | CC(C)(C)[Si](C)(C)OC(=O)C1CCCCC1   |
| <b>Mol. weight [g/mol]:</b> | 242.43   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.83   |      | Crippen Method |
| logp          | 4.115   |      | Crippen Method |
| rinpol        | 1410.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R65520&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R65520&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                               |

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/40-216-7/Cyclohexanecarboxylic-acid-DMTBS.pdf>

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