

Decanoic acid, tert-butyldimethylsilyl ester

Other names:

Decanoic acid, DMTBS
Decanoic acid, TBDMS
Capric acid, TBDMS
Capric acid, DMTBS
tert-Butyl(dimethyl)silyl decanoate
Decanoic acid, tbdms derivative

Inchi:

InChI=1S/C16H34O2Si/c1-7-8-9-10-11-12-13-14-15(17)18-19(5,6)16(2,3)4/h7-14H2,1-6H1

InchiKey:

RHAJQGDSFGQRLC-UHFFFAOYSA-N

Formula:

C₁₆H₃₄O₂Si

SMILES:

CCCCCCCCC(=O)O[Si](C)(C)C(C)C

Mol. weight [g/mol]:

286.53

CAS:

104255-74-5

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.43 | | Crippen Method |
| logp | 5.676 | | Crippen Method |
| rinpol | 1681.30 | | NIST Webbook |
| rinpol | 1674.00 | | NIST Webbook |
| rinpol | 1685.00 | | NIST Webbook |
| rinpol | 1684.00 | | NIST Webbook |
| rinpol | 1674.00 | | NIST Webbook |
| rinpol | 1685.00 | | NIST Webbook |
| ripol | 1777.00 | | NIST Webbook |
| ripol | 1777.00 | | NIST Webbook |

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255745&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/22-492-1/Decanoic-acid-tert-butyl-dimethylsilyl-ester.pdf>

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