

cis-10-Heptadecenoic acid, tert-butyldimethylsilyl ester

Other names: 10-Heptadecenoic acid, (z)-, tbdms derivative
Inchi: InChI=1S/C23H46O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(24)25-26(5,6)
InchiKey: JVNKZFLVPRCQNG-SEYXRHQNSA-N
Formula: C23H46O2Si
SMILES: CCCCCC=CCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 382.70

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -6.22 | | Crippen Method |
| logp | 8.182 | | Crippen Method |
| rinpol | 2373.90 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333625&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

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<https://www.chemeo.com/cid/36-868-9/cis-10-Heptadecenoic-acid-tert-butyldimethylsilyl-ester.pdf>

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