

# Heptadecanoic acid, tert-butyldimethylsilyl ester

**Other names:**

Heptadecanoic acid, TBDMS

Margaric acid, TBDMS ester

Margaric acid, TBDMS

Margarate, TBDMS

Margaric acid, DMTBS

Heptadecanoic acid, tbdms derivative

**Inchi:** InChI=1S/C23H48O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(24)25-26(5,6)**InchiKey:** PADPNPKFJSPJIC-UHFFFAOYSA-N**Formula:** C<sub>23</sub>H<sub>48</sub>O<sub>2</sub>Si**SMILES:** CCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C**Mol. weight [g/mol]:** 384.71**CAS:** 104255-81-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	8.406		Crippen Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2387.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2373.00		NIST Webbook
rinpol	2388.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255814&Units=SI>

# Legend

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

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