

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:** C₂₃H₄₈O₂Si**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	2387.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2373.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2388.00		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**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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