

Undecanoic acid, tert-butyldimethylsilyl ester

Other names: Undecanoic acid, TBDMS
Undecanoic acid, DMTBS
Undecanoic acid, tbdms derivative

Inchi: InChI=1S/C17H36O2Si/c1-7-8-9-10-11-12-13-14-15-16(18)19-20(5,6)17(2,3)4/h7-15H2,1

InchiKey: IJPQNIPLGFIDLM-UHFFFAOYSA-N

Formula: C17H36O2Si

SMILES: CCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 300.55

CAS: 104255-75-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	6.066		Crippen Method
rinpol	1781.60		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1773.00		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=C104255756&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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