

Tropic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester

Other names:	Tropic acid, TBDMS Tropic acid, bis-TBDMS Tropate, TBDMS Tropic acid, 2tdms derivative
Inchi:	InChI=1S/C21H38O3Si2/c1-20(2,3)25(7,8)23-16-18(17-14-12-11-13-15-17)19(22)24-26(
InchiKey:	DMPHHMWSYJVBNE-UHFFFAOYSA-N
Formula:	C21H38O3Si2
SMILES:	CC(C)(C)[Si](C)(C)OCC(C(=O)O[Si](C)(C)C(C)(C)C)c1ccccc1
Mol. weight [g/mol]:	394.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	6.340		Crippen Method
rinpol	2033.00		NIST Webbook
rinpol	2011.40		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2033.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352438&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.cheméo.com/cid/23-364-2/Tropic-acid-tert-butyltrimethylsilyl-ether-tert-butyltrimethylsilyl-ester.pdf>

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