

1-Dodecanol, O-TBDMS

Inchi:	InChI=1S/C18H40OSi/c1-7-8-9-10-11-12-13-14-15-16-17-19-20(5,6)18(2,3)4/h7-17H2,1-
InchiKey:	NMTUSPFSWYXRJN-UHFFFAOYSA-N
Formula:	C18H40OSi
SMILES:	CCCCCCCCCCCCO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	300.60
CAS:	114058-22-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	6.929		Crippen Method
rinpol	1800.00		NIST Webbook
rinpol	1783.30		NIST Webbook
rinpol	1784.20		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1783.30		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1762.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C114058229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

rinpol: Non-polar retention indices

ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/89-134-5/1-Dodecanol-O-TBDMS.pdf>

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