1-Pentanol, 3,4-dimethyl, TMS

Inchi:	InChI=1S/C10H24OSi/c1-9(2)10(3)7-8-11-12(4,5)6/h9-10H,7-8H2,1-6H3
InchiKey:	PTQMCIYBLKCYNE-UHFFFAOYSA-N
Formula:	C10H24OSi
SMILES:	CC(C)C(C)CCO[Si](C)(C)C
Mol. weight [g/mol]:	188.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.66		Crippen Method
logp	3.520		Crippen Method
rinpol	1035.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R119407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

https://www.chemeo.com/cid/28-718-4/1-Pentanol-3-4-dimethyl-TMS.pdf

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