

# Creatinine, TBDMS

<b>Inchi:</b>	InChI=1S/C22H49N3OSi3/c1-20(2,3)27(11,12)23-19-24(10)17-18(26-29(15,16)22(7,8)9)
<b>InchiKey:</b>	DEPGDXVFUGKKQF-UHFFFAOYSA-N
<b>Formula:</b>	C22H49N3OSi3
<b>SMILES:</b>	Cn1cc(O[Si](C)(C)C(C)(C)C)n([Si](C)(C)C(C)(C)C)c1=N[Si](C)(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	455.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	6.970		Crippen Method
rinpol	1941.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R276758&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R276758&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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<https://www.chemeo.com/cid/67-921-5/Creatinine-TBDMS.pdf>

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