

Creatinine, TMS

Inchi: InChI=1S/C10H23N3OSi2/c1-13-8-9(14-16(5,6)7)11-10(13)12-15(2,3)4/h8H2,1-7H3/b12-
InchiKey: VRTXDBYUEQGXBD-ZRDIBKRKSA-N
Formula: C10H23N3OSi2
SMILES: CN1CC(O[Si](C)(C)C)=NC1=N[Si](C)(C)C
Mol. weight [g/mol]: 257.48

Physical Properties

Property code	Value	Unit	Source
log10ws	2.52		Crippen Method
logp	2.373		Crippen Method
rinsol	1570.00		NIST Webbook
rinsol	1570.00		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=R5195&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/31-384-1/Creatinine-TMS.pdf>

Generated by Cheméo on 2024-05-03 10:08:03.612494961 +0000 UTC m=+17020132.533072275.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.