

d3-creatinine, tri-TMS

Inchi: InChI=1S/C13H31N3OSi3/c1-15-11-12(17-20(8,9)10)16(19(5,6)7)13(15)14-18(2,3)4/h11
InchiKey: LZKCXGZZEBFBHI-MUFUOGHMSA-N
Formula: C13H28D3N3OSi3
SMILES: Cn1cc(O[Si](C)(C)C)n([Si](C)(C)C)c1=N[Si](C)(C)C
Mol. weight [g/mol]: 332.68

Physical Properties

Property code	Value	Unit	Source
log10ws	1.35		Crippen Method
logp	3.459		Crippen Method
rinpol	1570.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R274772&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/37-884-0/d3-creatinine-tri-TMS.pdf>

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