

deoxyinosine, TMS

Inchi: InChI=1S/C19H36N4O4Si3/c1-28(2,3)24-11-15-14(26-29(4,5)6)10-16(25-15)23-13-22-17
InchiKey: KSBDCWUOIDXEOA-UHFFFAOYSA-N
Formula: C19H36N4O4Si3
SMILES: C[Si](C)(C)OCC1OC(n2cnc3c(O[Si](C)(C)C)ncnc32)CC1O[Si](C)(C)C
Mol. weight [g/mol]: 468.77

Physical Properties

Property code	Value	Unit	Source
log10ws	0.45		Crippen Method
logp	4.399		Crippen Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R207113&Units=SI>

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/121-559-7/deoxyinosine-TMS.pdf>

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