

2'-Deoxyinosine, tris(trimethylsilyl) derivative

Inchi: InChI=1S/C19H36N4O4Si3/c1-28(2,3)23-13-21-18-17(19(23)24)20-12-22(18)16-10-14(2)
InchiKey: OBICRJNXWBSLIC-UHFFFAOYSA-N
Formula: C19H36N4O4Si3
SMILES: C[Si](C)(C)OCC1OC(n2cnc3c(=O)n([Si](C)(C)C)cnc32)CC1O[Si](C)(C)C
Mol. weight [g/mol]: 468.77

Physical Properties

Property code	Value	Unit	Source
log10ws	1.46		Crippen Method
logp	3.635		Crippen Method
rinpol	2545.50		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332822&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/50-972-7/2-Deoxyinosine-tris-trimethylsilyl-derivative.pdf>

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