

2'-Deoxyinosine, tris(tert-butyldimethylsilyl) derivative

Inchi: InChI=1S/C28H54N4O4Si3/c1-26(2,3)37(10,11)32-19-30-24-23(25(32)33)29-18-31(24)2
InchiKey: OHNDCCPWVMKBGW-UHFFFAOYSA-N
Formula: C28H54N4O4Si3
SMILES: CC(C)(C)[Si](C)(C)OCC1OC(n2cnc3c(=O)n([Si](C)(C)C(C)(C)C)cnc32)CC1O[Si](C)(C)C
Mol. weight [g/mol]: 595.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	7.146		Crippen Method
rinpol	3627.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332821&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/52-986-0/2-Deoxyinosine-tris-tert-butyldimethylsilyl-derivative.pdf>

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