

Cytosine arabinoside, methyl-TMS derivative

Inchi: InChI=1S/C22H47N3O5Si4/c1-24(31(2,3)4)18-14-15-25(22(26)23-18)21-20(30-34(11,12)35)32-29-33-36-37-38-39-40-41-42
InchiKey: DWWKRXKBASGMCZ-VWEINGBSSA-N
Formula: C22H47N3O5Si4
SMILES: CN(c1ccn(C2OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C)c(=O)n1)[Si](C)(C)C
Mol. weight [g/mol]: 545.97

Physical Properties

Property code	Value	Unit	Source
log10ws	4.07		Crippen Method
logp	4.703		Crippen Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R245848&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/43-134-5/Cytosine-arabinoside-methyl-TMS-derivative.pdf>

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