

trans-5-hydroxypipicolinic acid, N(O,S)-isoBOC TBDMS

Inchi: InChI=1S/C22H41NO7Si/c1-15(2)13-27-20(25)23-12-17(29-21(26)28-14-16(3)4)10-11-18
InchiKey: OXONXQHBFUTZAY-ZWKOTPCHSA-N
Formula: C22H41NO7Si
SMILES: CC(C)COC(=O)OC1CCC(C(=O)O[Si](C)(C)C(C)(C)C)N(C(=O)OCC(C)C)C1
Mol. weight [g/mol]: 459.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	4.970		Crippen Method
rinpol	2171.90		NIST Webbook
rinpol	2171.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R522511&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/51-835-8/trans-5-hydroxypipicolinic-acid-N-O-S-isoBOC-TBDMS.pdf>

Generated by Cheméo on 2025-12-05 08:21:15.380753283 +0000 UTC m=+4671072.910793939.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.