

Imidazole-5-lactic acid, TMS

Inchi: InChI=1S/C15H32N2O3Si3/c1-21(2,3)17-12-16-11-13(17)10-14(19-22(4,5)6)15(18)20-23
InchiKey: YQHNOGLELKHYKS-UHFFFAOYSA-N
Formula: C15H32N2O3Si3
SMILES: C[Si](C)(C)OC(=O)C(Cc1cncn1[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 372.68

Physical Properties

Property code	Value	Unit	Source
log10ws	2.53		Crippen Method
logp	3.707		Crippen Method
rinpol	1787.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94884&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/10-418-6/Imidazole-5-lactic-acid-TMS.pdf>

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