

Imidazole-4,5-dicarboxylic acid, TMS

Inchi: InChI=1S/C14H28N2O4Si3/c1-21(2,3)16-10-15-11(13(17)19-22(4,5)6)12(16)14(18)20-23
InchiKey: MIQWKSYPARCWNTR-UHFFFAOYSA-N
Formula: C14H28N2O4Si3
SMILES: C[Si](C)(C)OC(=O)c1ncn([Si](C)(C)C)c1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 372.64

Physical Properties

Property code	Value	Unit	Source
log10ws	2.16		Crippen Method
logp	3.549		Crippen Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94866&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/119-218-8/Imidazole-4-5-dicarboxylic-acid-TMS.pdf>

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