

4-Aminoimidazole-5-carboxamide, TMS

Inchi: InChI=1S/C13H30N4OSi3/c1-19(2,3)15-12-11(13(18)16-20(4,5)6)17(10-14-12)21(7,8)9/h
InchiKey: SDNCHTLQCKEOED-UHFFFAOYSA-N
Formula: C13H30N4OSi3
SMILES: C[Si](C)(C)NC(=O)c1c(N[Si](C)(C)C)ncn1[Si](C)(C)C
Mol. weight [g/mol]: 342.66

Physical Properties

Property code	Value	Unit	Source
log10ws	2.30		Crippen Method
logp	3.378		Crippen Method
rinpol	1811.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93711&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/30-942-2/4-Aminoimidazole-5-carboxamide-TMS.pdf>

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