

Imidazole-5-acetic acid, TMS

Inchi: InChI=1S/C11H22N2O2Si2/c1-16(2,3)13-9-12-8-10(13)7-11(14)15-17(4,5)6/h8-9H,7H2,1
InchiKey: YNWZDALAZNSOJV-UHFFFAOYSA-N
Formula: C11H22N2O2Si2
SMILES: C[Si](C)(C)OC(=O)Cc1cncn1[Si](C)(C)C
Mol. weight [g/mol]: 270.48

Physical Properties

Property code	Value	Unit	Source
log10ws	1.45		Crippen Method
logp	2.487		Crippen Method
rinpol	1501.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94870&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/42-020-2/Imidazole-5-acetic-acid-TMS.pdf>

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