

13C5-PROLINE (TMS)

Inchi: InChI=1S/C11H25NO2Si2/c1-15(2,3)12-9-7-8-10(12)11(13)14-16(4,5)6/h10H,7-9H2,1-6H
InchiKey: DKGIXVJPGFXLRM-QBZHADDCSA-N
Formula: C11H25NO2Si2
SMILES: C[Si](C)(C)OC(=O)C1CCCN1[Si](C)(C)C
Mol. weight [g/mol]: 259.49

Physical Properties

Property code	Value	Unit	Source
log10ws	2.03		Crippen Method
logp	2.664		Crippen Method
rinpol	1301.70		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R414896&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/16-484-7/13C5-PROLINE-TMS.pdf>

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