

Proline, MTH-TMS

Inchi: InChI=1S/C10H18N2OSSi/c1-11-9(13-15(2,3)4)8-6-5-7-12(8)10(11)14/h5-7H2,1-4H3
InchiKey: RPBYPGCGSGATCG-UHFFFAOYSA-N
Formula: C10H18N2OSSi
SMILES: Cn1c(O[Si](C)(C)C)c2n(c1=S)CCC2
Mol. weight [g/mol]: 242.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.716		Crippen Method
rinpol	1543.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525496&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/28-781-4/Proline-MTH-TMS.pdf>

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