

Citrulline, TMS

Inchi: InChI=1S/C15H37N3O3Si3/c1-22(2,3)17-13(14(19)21-24(7,8)9)11-10-12-16-15(20)18-23
InchiKey: XPPZURUXPNOCEH-CYBMUJFWSA-N
Formula: C15H37N3O3Si3
SMILES: C[Si](C)(C)NC(=O)NCCCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 391.73

Physical Properties

Property code	Value	Unit	Source
log10ws	2.45		Crippen Method
logp	3.072		Crippen Method
rinpol	1836.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94496&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/68-738-8/Citrulline-TMS.pdf>

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