

Tyramine, iso-BOC, O-TBDMS

Inchi: InChI=1S/C19H33NO3Si/c1-15(2)14-22-18(21)20-13-12-16-8-10-17(11-9-16)23-24(6,7)1
InchiKey: KGEHPSQB-YAFMLB-UHFFFAOYSA-N
Formula: C₁₉H₃₃NO₃Si
SMILES: CC(C)COC(=O)NCCc1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 351.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	4.995		Crippen Method
rinpol	2461.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R392880&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/113-374-1/Tyramine-iso-BOC-O-TBDMS.pdf>

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