

Tyrosine, MTH-TMS

Inchi: InChI=1S/C17H28N2O2SSi2/c1-19-16(21-24(5,6)7)15(18-17(19)22)12-13-8-10-14(11-9-
InchiKey: MZLMUYFDCGMWRO-UHFFFAOYSA-N
Formula: C17H28N2O2SSi2
SMILES: Cn1c(O[Si](C)(C)C)c(Cc2ccc(O[Si](C)(C)C)cc2)[nH]c1=S
Mol. weight [g/mol]: 380.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	4.619		Crippen Method
rinpol	2343.00		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=R525530&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/64-563-6/Tyrosine-MTH-TMS.pdf>

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