

L-Tyrosine, N,O-bis(trimethylsilyl)-, trimethylsilyl ester

Other names:

Tyrosine, (3TMS)

Tyrosine, tri-TMS

Tyr, (N,O,O-TMS)

Tyr, TMS

TYROSINE (N,O,O-TMS)

Tyrosine, TMS

L-tyrosine, 3tms derivative

Inchi: InChI=1S/C18H35NO3Si3/c1-23(2,3)19-17(18(20)22-25(7,8)9)14-15-10-12-16(13-11-15)

InchiKey: WMWBCQXPKSQMOK-QGZVFWFLSA-N

Formula: C18H35NO3Si3

SMILES: C[Si](C)(C)NC(Cc1ccc(O[Si](C)(C)C)cc1)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 397.73

CAS: 51220-73-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.52		Crippen Method
logp	4.614		Crippen Method
rinpol	1950.38		NIST Webbook
rinpol	1960.08		NIST Webbook
rinpol	1959.22		NIST Webbook
rinpol	1954.20		NIST Webbook
rinpol	1964.36		NIST Webbook
rinpol	1937.10		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1949.42		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1928.50		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1949.42		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1952.00		NIST Webbook
ripol	2151.59		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C51220736&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
ripol: Polar retention indices

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