

L-Tryptophan, N,1-bis(trimethylsilyl)-, trimethylsilyl ester

Other names:

L-Tryptophan, N,N'-trimethylsilyl-, trimethylsilyl ester

Trp, (N,N,O-tris-TMS)

Tryptophan, N,N,O-triTMS

Trp, TMS

TRYPTOPHANE (N,N,O-TMS)

TRYPTOPHAN,N,N,O-TMS

L-tryptophan, 3tms derivative

Inchi: InChI=1S/C20H36N2O2Si3/c1-25(2,3)21-18(20(23)24-27(7,8)9)14-16-15-22(26(4,5)6)19

InchiKey: JRAGJGVCQZJQIM-SFHVURJKSA-N

Formula: C20H36N2O2Si3

SMILES: C[Si](C)(C)NC(Cc1cn([Si](C)(C)C)c2cccc12)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 420.77

CAS: 55429-28-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.39		Crippen Method
logp	5.038		Crippen Method
rinpol	2208.39		NIST Webbook
rinpol	2235.62		NIST Webbook
rinpol	2208.30		NIST Webbook
rinpol	2214.50		NIST Webbook
rinpol	2235.62		NIST Webbook
rinpol	2208.39		NIST Webbook
rinpol	2218.50		NIST Webbook
rinpol	2214.50		NIST Webbook
rinpol	2208.30		NIST Webbook
rinpol	2237.31		NIST Webbook
rinpol	2218.50		NIST Webbook
ripol	2548.52		NIST Webbook
ripol	2548.52		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55429282&Units=SI>

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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