

7-Carboxyheptanoylglycine di-O-tms

Other names: Suberylglycine, TMS # 1
Suberylglycine, diTMS

Inchi: InChI=1S/C16H33NO5Si2/c1-23(2,3)21-15(19)12-10-8-7-9-11-14(18)17-13-16(20)22-24

InchiKey: HZXUKAOEDBVOKB-UHFFFAOYSA-N

Formula: C16H33NO5Si2

SMILES: C[Si](C)(C)OC(=O)CCCCC(=O)NCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 375.61

Physical Properties

Property code	Value	Unit	Source
log10ws	0.69		Crippen Method
logp	3.199		Crippen Method
rinpol	2026.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2026.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U102889&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/124-325-3/7-Carboxyheptanoylglycine-di-O-tms.pdf>

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