

2-Trimethylsilyloxysebacic acid, bis(trimethylsilyl)- ester

Other names:

Decanedioic acid, «alpha»-TMS ether, TMS ester

2-Hydroxysebacic acid, triTMS

Inchi:

InChI=1S/C19H42O5Si3/c1-25(2,3)22-17(19(21)24-27(7,8)9)15-13-11-10-12-14-16-18(20)

InchiKey:

ASPGPTJHUAATH-UHFFFAOYSA-N

Formula:

C19H42O5Si3

SMILES:

C[Si](C)(C)OC(=O)CCCCCCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

434.79

Physical Properties

Property code	Value	Unit	Source
log10ws	1.15		Crippen Method
logp	5.693		Crippen Method
rinpol	2059.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U79059&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

Latest version available from:

<https://www.chemeo.com/cid/28-045-1/2-Trimethylsilyloxysebacic-acid-bis-trimethylsilyl-ester.pdf>

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