

Nonanedioic acid, bis(tert-butyldimethylsilyl) ester

Other names:

Azelaic acid, bis(tert-butyldimethylsilyl) ester

Azelaic acid, diTBDMS

Nonanedioic acid, bis-TBDMS ester

Nonanedioic acid, TBDMS

Bis[tert-butyl(dimethyl)silyl] azelaate

Azelaic acid, 2tbdms derivative

Inchi: InChI=1S/C21H44O4Si2/c1-20(2,3)26(7,8)24-18(22)16-14-12-11-13-15-17-19(23)25-27(24)

InchiKey: VVOJIMXLEIRYGX-UHFFFAOYSA-N

Formula: C₂₁H₄₄O₄Si₂

SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 416.74

CAS: 104255-97-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	6.814		Crippen Method
rinpol	2278.00		NIST Webbook
rinpol	2263.10		NIST Webbook
rinpol	2272.47		NIST Webbook
rinpol	2272.47		NIST Webbook

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255972&Units=SI>

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.cheméo.com/cid/52-854-6/Nonanedioic-acid-bis-tert-butyltrimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-25 07:29:54.043009941 +0000 UTC m=+16319442.963587257.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.