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(

InchiKey: VVOJIMXLEIRYGX-UHFFFAOYSA-N

Formula: C21H44O4Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCCCCCCC(=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/ci990307l

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