

Nonadecanoic acid, tert-butyldimethylsilyl ester

Other names:

Nonadecanoic acid, TBDMS
tert-Butyl(dimethyl)silyl nonadecanoate
Nonadecanoic acid, tbdms derivative

Inchi:

InChI=1S/C25H52O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24(26)27-

InchiKey:

IRJWTOHPSQRGKW-UHFFFAOYSA-N

Formula:

C₂₅H₅₂O₂Si

SMILES:

CCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]:

412.76

CAS:

104255-82-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.20		Crippen Method
logp	9.186		Crippen Method
rinpol	2583.80		NIST Webbook
rinpol	2589.00		NIST Webbook
rinpol	2576.00		NIST Webbook
rinpol	2583.80		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=C104255825&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/57-086-4/Nonadecanoic-acid-tert-butyl-dimethylsilyl-ester.pdf>

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