

trans-Vaccenic acid, tert-butyldimethylsilyl ester

Other names:	Vaccenic acid, (e)-, tbdms derivative
Inchi:	InChI=1S/C24H48O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(25)26-27(
InchiKey:	ZYXNQUCAMMMNNE-OUKQBFOZSA-N
Formula:	C24H48O2Si
SMILES:	CCCCCCC=CCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	396.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	8.572		Crippen Method
rinpol	2473.30		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/22-096-1/trans-Vaccenic-acid-tert-butyldimethylsilyl-ester.pdf>

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