

3-Phenyllactic acid, TBDMS

Other names:	DL-3-Phenyllactic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester 3-Phenyllactic acid, TBDMS Phenyllactic acid, TBDMS
Inchi:	InChI=1S/C21H38O3Si2/c1-20(2,3)25(7,8)23-18(16-17-14-12-11-13-15-17)19(22)24-26(
InchiKey:	JFLMDZUHGCHDPN-UHFFFAOYSA-N
Formula:	C21H38O3Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C(Cc1ccccc1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	394.70

Physical Properties

Property code	Value	Unit	Source
logp	6.168		Crippen Method
rinpol	2031.10		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2016.00		NIST Webbook
tb	591.36	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89682031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.cheméo.com/cid/68-658-7/3-Phenyllactic-acid-TBDMS.pdf>

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