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(9
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/ci990307l

Legend

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