4-Butyl-1-phenyl-pyrazolidine-3,5-diol, O,O'-bis(tert-butyldimethylsilyl) ether

Other names: 4-Butyl-1-phenyl-pyrazolidine-3,5-dione 2tBDMS
Inchi: InChI=1S/C25H44N2O2Si2/c1-12-13-19-21-22(28-30(8,9)24(2,3)4)26-27(20-17-15-14-16
InchiKey: BLSNHECDXZNEIH-UHFFFAOYSA-N
Formula: C25H44N2O2Si2
SMILES: CCCCc1c(O[Si](C)(C)C(C)(C)C)nn(-c2ccccc2)c1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 460.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	7.983		Crippen Method
rinpol	2446.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373392&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices