

(1R2R)-Ephedrine, N-(2-phenylbutanoyl)-O-TMS

Inchi: InChI=1S/C23H33NO2Si/c1-7-21(19-14-10-8-11-15-19)23(25)24(3)18(2)22(26-27(4,5)6)
InchiKey: WKCMQVCLOHXYPJ-IDTFUIECSA-N
Formula: C23H33NO2Si
SMILES: CCC(C(=O)N(C)C(C)C(O[Si](C)(C)C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 383.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	5.620		Crippen Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R99307&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

Latest version available from:

<https://www.chemeo.com/cid/11-246-6/1R2R-Ephedrine-N-2-phenylbutanoyl-O-TMS.pdf>

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