

Epinephrine, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C32H63NO5Si3/c1-24(2)23-35-29(34)33(12)22-28(38-41(17,18)32(9,10)11)25
InchiKey: FYJTUNFGOZGXOW-UHFFFAOYSA-N
Formula: C32H63NO5Si3
SMILES: CC(C)COC(=O)N(C)CC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 626.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	10.242		Crippen Method
rinpol	3172.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R392464&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/117-081-2/Epinephrine-N-isoBOC-O-TBDMS.pdf>

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