

# Adrenaline, DTFMB-TBDMS

**Inchi:** InChI=1S/C36H57F6NO4Si3/c1-32(2,3)48(11,12)45-28-18-17-24(21-29(28)46-49(13,14))  
**InchiKey:** UMDBQTBNTLUKHK-UHFFFAOYSA-N  
**Formula:** C36H57F6NO4Si3  
**SMILES:** CN(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)c1)C(=O)C  
**Mol. weight [g/mol]:** 766.09

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	12.327		Crippen Method
rinpol	3022.00		NIST Webbook
rinpol	3022.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R54068&Units=SI>

## 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/114-137-3/Adrenaline-DTFMB-TBDMS.pdf>

Generated by Cheméo on 2024-04-28 03:22:24.031530661 +0000 UTC m=+16563792.952107974.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.