

# Adrenaline, N-HFB-O-TMS

**Inchi:** InChI=1S/C22H36F7NO4Si3/c1-30(19(31)20(23,24)21(25,26)22(27,28)29)14-18(34-37(8  
**InchiKey:** YGLMMYJNTVLKEX-UHFFFAOYSA-N  
**Formula:** C22H36F7NO4Si3  
**SMILES:** CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)C(F)(F)C(F)(F)C(F)(F)  
**Mol. weight [g/mol]:** 595.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Crippen Method
logp	7.298		Crippen Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook

## Sources

**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=R139154&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## Legend

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

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<https://www.chemeo.com/cid/116-080-4/Adrenaline-N-HFB-O-TMS.pdf>

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