

Adrenaline, N-DTFMB-TMS

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|-----------------------------|---|
| Other names: | Adrenaline, DTFMB-TMS |
| Inchi: | InChI=1S/C27H39F6NO4Si3/c1-34(25(35)19-13-20(26(28,29)30)16-21(14-19)27(31,32)3 |
| InchiKey: | PGCARAXUUGXVRZ-UHFFFAOYSA-N |
| Formula: | C27H39F6NO4Si3 |
| SMILES: | CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1 |
| Mol. weight [g/mol]: | 639.85 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.72 | | Crippen Method |
| logp | 8.816 | | Crippen Method |
| rinpola | 2386.00 | | NIST Webbook |
| rinpola | 2386.00 | | NIST Webbook |
| rinpola | 2386.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R164942&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 |
| rinpola: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/58-792-9/Adrenaline-N-DTFMB-TMS.pdf>

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