

sumatriptan, TMS

Inchi: InChI=1S/C20H37N3O2SSi2/c1-21(2)13-12-18-15-23(28(7,8)9)20-11-10-17(14-19(18)20)
InchiKey: NEWUXABEIGAUTL-UHFFFAOYSA-N
Formula: C20H37N3O2SSi2
SMILES: CN(C)CCc1cn([Si](C)(C)C)c2ccc(CS(=O)(=O)N(C)[Si](C)(C)C)cc12
Mol. weight [g/mol]: 439.76

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.82 | | Crippen Method |
| logp | 4.025 | | Crippen Method |
| rinpol | 2800.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299286&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/30-332-9/sumatriptan-TMS.pdf>

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