

1-isopropyl,3,7,10-trimethylsilatrane, d

Inchi: InChI=1S/C12H25NO3Si/c1-9(2)17-14-10(3)6-13(7-11(4)15-17)8-12(5)16-17/h9-12H,6-8
InchiKey: MFNQPKFQWOSBLY-UHFFFAOYSA-N
Formula: C12H25NO3Si
SMILES: CC1CN2CC(C)O[Si](C(C)C)(O1)OC(C)C2
Mol. weight [g/mol]: 259.42

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.02 | | Crippen Method |
| logp | 1.880 | | Crippen Method |
| rinpol | 1410.00 | | NIST Webbook |
| rinpol | 1410.00 | | NIST Webbook |
| ripol | 1903.00 | | NIST Webbook |
| ripol | 1903.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R145718&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
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-966-5/1-isopropyl-3-7-10-trimethylsilatrane-d.pdf>

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