

cis-5-Dodecenoic acid, dimethyl(3,3,3-trifluoropropyl)silyl ester

Inchi: InChI=1S/C17H31F3O2Si/c1-4-5-6-7-8-9-10-11-12-13-16(21)22-23(2,3)15-14-17(18,19)2
InchiKey: OCOYVVOZIHDCLEF-KTKRTIGZSA-N
Formula: C17H31F3O2Si
SMILES: CCCCCC=CCCC(=O)O[Si](C)(C)CC(F)(F)F
Mol. weight [g/mol]: 352.51

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.37 | | Crippen Method |
| logp | 6.384 | | Crippen Method |
| rinpol | 1735.00 | | NIST Webbook |
| rinpol | 1735.00 | | 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=U375597&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/116-529-6/cis-5-Dodecenoic-acid-dimethyl-3-3-3-trifluoropropyl-silyl-ester.pdf>

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