

Cystine, tri-TMS

Inchi: InChI=1S/C15H36N2O4S2Si3/c1-24(2,3)17-13(15(19)21-26(7,8)9)11-23-22-10-12(16)14
InchiKey: NIRWUGJVFWNGAW-UHFFFAOYSA-N
Formula: C15H36N2O4S2Si3
SMILES: C[Si](C)(C)NC(CSSCC(N)C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 456.84

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 2.42 | | Crippen Method |
| logp | 3.244 | | Crippen Method |
| rinpol | 2319.00 | | NIST Webbook |
| rinpol | 2319.00 | | 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=R330164&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/57-432-9/Cystine-tri-TMS.pdf>

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