

Citric acid 3TMS

Inchi: InChI=1S/C15H32O7Si3/c1-23(2,3)20-12(16)10-15(19,14(18)22-25(7,8)9)11-13(17)21-24
InchiKey: HNRUOTSRMGCNPS-UHFFFAOYSA-N
Formula: C15H32O7Si3
SMILES: C[Si](C)(C)OC(=O)CC(O)(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 408.67
CAS: 1327339-35-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 3.78 | | Crippen Method |
| logp | 2.632 | | Crippen Method |
| rinpola | 1767.40 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1327339354&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpola: Non-polar retention indices

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<https://www.cheméo.com/cid/75-160-1/Citric-acid-3TMS.pdf>

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