

Levoglucozan, pyranose, TMS

Inchi: InChI=1S/C15H34O5Si3/c1-21(2,3)18-12-11-10-16-15(17-11)14(20-23(7,8)9)13(12)19-2
InchiKey: OEPKLYQQZLBNKR-BTFPBAQTSA-N
Formula: C15H34O5Si3
SMILES: C[Si](C)(C)OC1C2COC(O2)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 378.68

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 3.47 | | Crippen Method |
| logp | 3.402 | | Crippen Method |
| rinsol | 1724.00 | | NIST Webbook |
| rinsol | 1724.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R517658&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/57-352-8/Levoglucozan-pyranose-TMS.pdf>

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