

# Psicose, acyclic, TMS

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | Psicose, TMS<br>D(+)-Talose, ketol, TMS                                          |
| Inchi:               | InChI=1S/C21H52O6Si5/c1-28(2,3)23-16-18(22)20(26-31(10,11)12)21(27-32(13,14)15)1 |
| InchiKey:            | LDUCAYFXHYLHLP-QHAWAJNXSA-N                                                      |
| Formula:             | C21H52O6Si5                                                                      |
| SMILES:              | C[Si](C)(C)OCC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C     |
| Mol. weight [g/mol]: | 541.06                                                                           |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 6.08    |      | Crippen Method |
| logp          | 5.919   |      | Crippen Method |
| rinpol        | 1838.00 |      | NIST Webbook   |
| rinpol        | 1838.00 |      | NIST Webbook   |
| rinpol        | 1872.00 |      | NIST Webbook   |
| rinpol        | 1872.00 |      | NIST Webbook   |
| ripol         | 1869.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R46025&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R46025&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |

## 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.cheméo.com/cid/71-169-6/Psicose-acyclic-TMS.pdf>

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