

A-Tagatofuranose, TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-18-19(25-30(7,8)9)20(26-31(10,11)12)21(24-15)3
InchiKey: PLNWQGWZBNJIQM-BQJUDKOJSA-N
Formula: C₂₁H₅₂O₆Si₅
SMILES: C[Si](C)(C)OCC1OC(CO[Si](C)(C)C)(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 541.06

Physical Properties

Property code	Value	Unit	Source
log10ws	5.77		Crippen Method
logp	6.076		Crippen Method
ripol	1721.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R45948&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
ripol: Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/71-168-7/A-Tagatofuranose-TMS.pdf>

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