

# Gentobiose, 8TMS

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| <b>Inchi:</b>    | InChI=1S/C36H86O11Si8/c1-48(2,3)38-26-28-30(42-50(7,8)9)31(43-51(10,11)12)33(45-53)34(46-54)35(47-55)36(49-56)37(52-57)39-41-44-40-27-29-32-35-58-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           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| <b>InchiKey:</b> | SWPQHIFGBMZXPV-LQAYEPCXSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         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| <b>Formula:</b>  | C36H86O11Si8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        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| <b>SMILES:</b>   | C[Si](C)(C)OCC1OC(OCC2OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C1OC3OC(OCC4OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4O[Si](C)(C)C3OC5OC(OCC6OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C6O[Si](C)(C)C5OC7OC(OCC8OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C8O[Si](C)(C)C7OC9OC(OCC10OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C10O[Si](C)(C)C9OC11OC(OCC12OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C12O[Si](C)(C)C11OC13OC(OCC14OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C14O[Si](C)(C)C13OC15OC(OCC16OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C16O[Si](C)(C)C15OC17OC(OCC18OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C18O[Si](C)(C)C17OC19OC(OCC20OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C20O[Si](C)(C)C19OC21OC(OCC22OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C22O[Si](C)(C)C21OC23OC(OCC24OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C24O[Si](C)(C)C23OC25OC(OCC26OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C26O[Si](C)(C)C25OC27OC(OCC28OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C28O[Si](C)(C)C27OC29OC(OCC30OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C30O[Si](C)(C)C29OC31OC(OCC32OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C32O[Si](C)(C)C31OC33OC(OCC34OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C34O[Si](C)(C)C33OC35OC(OCC36OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C36O[Si](C)(C)C35OC37OC(OCC38OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C38O[Si](C)(C)C37OC39OC(OCC40OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C40O[Si](C)(C)C39OC41OC(OCC42OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C42O[Si](C)(C)C41OC43OC(OCC44OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C44O[Si](C)(C)C43OC45OC(OCC46OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C46O[Si](C)(C)C45OC47OC(OCC48OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C48O[Si](C)(C)C47OC49OC(OCC50OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C50O[Si](C)(C)C49OC51OC(OCC52OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C52O[Si](C)(C)C51OC53OC(OCC54OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C54O[Si](C)(C)C53OC55OC(OCC56OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C56O[Si](C)(C)C55OC57OC(OCC58OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C58O[Si](C)(C)C57OC59OC(OCC60OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C60O[Si](C)(C)C59OC61OC(OCC62OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C62O[Si](C)(C)C61OC63OC(OCC64OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C64O[Si](C)(C)C63OC65OC(OCC66OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C66O[Si](C)(C)C65OC67OC(OCC68OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C68O[Si](C)(C)C67OC69OC(OCC70OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C70O[Si](C)(C)C69OC71OC(OCC72OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C72O[Si](C)(C)C71OC73OC(OCC74OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C74O[Si](C)(C)C73OC75OC(OCC76OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C76O[Si](C)(C)C75OC77OC(OCC78OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C78O[Si](C)(C)C77OC79OC(OCC80OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C80O[Si](C)(C)C79OC81OC(OCC82OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C82O[Si](C)(C)C81OC83OC(OCC84OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C84O[Si](C)(C)C83OC85OC(OCC86OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C86O[Si](C)(C)C85OC87OC(OCC88OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C88O[Si](C)(C)C87OC89OC(OCC90OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C90O[Si](C)(C)C89OC91OC(OCC92OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C92O[Si](C)(C)C91OC93OC(OCC94OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C94O[Si](C)(C)C93OC95OC(OCC96OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C96O[Si](C)(C)C95OC97OC(OCC98OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C98O[Si](C)(C)C97OC99OC(OCC100OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C100O[Si](C)(C)C99OC101OC(OCC102OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C102O[Si](C)(C)C101OC103OC(OCC104OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C104O[Si](C)(C)C103OC105OC(OCC106OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C106O[Si](C)(C)C105OC107OC(OCC108OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C108O[Si](C)(C)C107OC109OC(OCC110OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C110O[Si](C)(C)C109OC111OC(OCC112OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C112O[Si](C)(C)C111OC113OC(OCC114OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C114O[Si](C)(C)C113OC115OC(OCC116OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C116O[Si](C)(C)C115OC117OC(OCC118OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C118O[Si](C)(C)C117OC119OC(OCC120OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C120O[Si](C)(C)C119OC121OC(OCC122OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C122O[Si](C)(C)C121OC123OC(OCC124OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C124O[Si](C)(C)C123OC125OC(OCC126OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C126O[Si](C)(C)C125OC127OC(OCC128OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C128O[Si](C)(C)C127OC129OC(OCC130OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C130O[Si](C)(C)C129OC131OC(OCC132OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C132O[Si](C)(C)C131OC133OC(OCC134OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C134O[Si |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 8.84    |      | Crippen Method |
| logp          | 9.476   |      | Crippen Method |
| rinpol        | 2828.00 |      | NIST Webbook   |
| rinpol        | 2828.00 |      | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R605760&Units=SI>

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>rinpol:</b>  | Non-polar retention indices         |

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