

Gentianose: bD-Gclp(1->6)-aDGlc(1->2)-DFru, oxime-TMS

Inchi: InChI=1S/C50H118O16Si11/c1-67(2,3)52-35-38-40(59-70(10,11)12)41(60-71(13,14)15)42-39-43-44-45-46-47-48-49
InchiKey: NJSRFQTYEVAEPI-XARCXXIWSA-N
Formula: C50H118O16Si11
SMILES: C[Si](C)(C)OCC1OC(OCC2OC(OC3(CO[Si](C)(C)C)OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C3)OC1
Mol. weight [g/mol]: 1284.40

Physical Properties

Property code	Value	Unit	Source
log10ws	12.06		Crippen Method
logp	12.837		Crippen Method
rinpol	3288.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R588833&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/116-939-1/Gentianose-bD-Gclp-1-6-aDGlc-1-2-DFru-oxime-TMS.pdf>

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