

2-O-(2-(4-hydroxyphenyl)-ethyl)-d-«beta»-glucopyranose-5TMS

InChI:
5TMS

InChI=1S/C29H60O7Si5/c1-37(2,3)31-22-25-26(34-39(7,8)9)27(35-40(10,11)12)28(29(30)32)33-36

InchiKey:

OFAVTKSDVWQTRU-UHFFFAOYSA-N

Formula:

C29H60O7Si5

SMILES:

C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(OCCc2ccc(O[Si](C)(C)C)cc2)C(O[Si](C)(C)C)C1O[Si](C)(C)C

Mol. weight [g/mol]:

661.21

CAS:

1036766-19-4

Physical Properties

Property code	Value	Unit	Source
log10ws	3.51		Crippen Method
logp	7.696		Crippen Method
rinsol	2741.50		NIST Webbook
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Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1036766194&Units=SI>

Legend

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

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