D-Psicose, pentakis(trimethylsilyl) ether, benzyloxime (isomer 2)

Inchi: InChI=1S/C28H59NO6Si5/c1-36(2,3)31-22-25(29-30-21-24-19-17-16-18-20-24)27(34-39

InchiKey: ILCMTPAXEPAWQO-UHFFFAOYSA-N

Formula: C28H59NO6Si5

SMILES: C[Si](C)(C)OCC(=NOCc1ccccc1)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](

Mol. weight [g/mol]: 646.20

Physical Properties

Property code	Value	Unit	Source
log10ws	3.59		Crippen Method
logp	7.922		Crippen Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380369&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/16-678-2/D-Psicose-pentakis-trimethylsilyl-ether-benzyloxime-isomer-2.pdf

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