

D-Psicose, pentakis(trimethylsilyl) ether, benzyloxime (isomer 1)

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](C)(C)C
Mol. weight [g/mol]: 646.20

Physical Properties

Property code	Value	Unit	Source
log10ws	3.59		Crippen Method
logp	7.922		Crippen Method
rinpol	2320.10		NIST Webbook
rinpol	2320.10		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U380368&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/41-819-7/D-Psicose-pentakis-trimethylsilyl-ether-benzyloxime-isomer-1.pdf>

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