

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

Inchi: InChI=1S/C28H59NO6Si5/c1-36(2,3)31-23-26(33-38(7,8)9)28(35-40(13,14)15)27(34-39)
InchiKey: HTPNKYHYJRZYRL-UHFFFAOYSA-N
Formula: C28H59NO6Si5
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C=NOCc1ccccc1)O[Si](C)(C)C
Mol. weight [g/mol]: 646.20

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 3.48 | | Crippen Method |
| logp | 7.921 | | Crippen Method |
| rinpol | 2411.90 | | NIST Webbook |

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=U380440&Units=SI>

Legend

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

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