

palatinitol 2, TMS

Inchi: InChI=1S/C39H96O11Si9/c1-51(2,3)41-29-31-34(46-55(13,14)15)37(49-58(22,23)24)38(59-60)1-2
InchiKey: MHRRBIHJBBEMLC-FTRYFTPOSA-N
Formula: C39H96O11Si9
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(COC1OC(CO[Si](C)(C)C)C1)C
Mol. weight [g/mol]: 993.94

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 10.04 | | Crippen Method |
| logp | 10.972 | | Crippen Method |
| rinpol | 3047.40 | | NIST Webbook |
| rinpol | 3047.40 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R489033&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/67-124-0/palatinitol-2-TMS.pdf>

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