

1,2-Dodecanediol, DTBS

Inchi: InChI=1S/C20H42O2Si/c1-8-9-10-11-12-13-14-15-16-18-17-21-23(22-18,19(2,3)4)20(5,6)
InchiKey: JMOBCXSEIOKGF0-UHFFFAOYSA-N
Formula: C20H42O2Si
SMILES: CCCCCCCCCC1CO[Si](C(C)(C)C)(C(C)(C)C)O1
Mol. weight [g/mol]: 342.63

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -5.01 | | Crippen Method |
| logp | 6.975 | | Crippen Method |
| rinpol | 2030.00 | | NIST Webbook |
| rinpol | 2030.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R115227&Units=SI>

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/95-724-3/1-2-Dodecanediol-DTBS.pdf>

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