

1,2-Propanediol, 3-(4-hydroxyphenyl), tris-TMS

Inchi: InChI=1S/C18H36O3Si3/c1-22(2,3)19-15-18(21-24(7,8)9)14-16-10-12-17(13-11-16)20-2
InchiKey: LUDKONSVLXFEHE-UHFFFAOYSA-N
Formula: C18H36O3Si3
SMILES: C[Si](C)(C)OCC(Cc1ccc(O[Si](C)(C)C)cc1)O[Si](C)(C)C
Mol. weight [g/mol]: 384.73

Physical Properties

Property code	Value	Unit	Source
log10ws	1.40		Crippen Method
logp	5.514		Crippen Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R99802&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/60-787-2/1-2-Propanediol-3-4-hydroxyphenyl-tris-TMS.pdf>

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