

GLUCOHEPTONIC ACID 7TMS

Inchi: InChI=1S/C28H70O8Si7/c1-37(2,3)30-22-23(31-38(4,5)6)24(32-39(7,8)9)25(33-40(10,11)
InchiKey: UPRYONQLEJIRBX-ZEEZOPKCSA-N
Formula: C28H70O8Si7
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(O[Si](C)(C)C)C(O[Si](C)(C)C)
Mol. weight [g/mol]: 731.45

Physical Properties

Property code	Value	Unit	Source
log10ws	8.15		Crippen Method
logp	8.316		Crippen Method
rincpol	2251.20		NIST Webbook
rincpol	2251.20		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=R414574&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-107-9/GLUCOHEPTONIC-ACID-7TMS.pdf>

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