

3,4-Dihydroxymandelic acid, TBDMS

Inchi: InChI=1S/C32H64O5Si4/c1-29(2,3)38(13,14)34-25-22-21-24(23-26(25)35-39(15,16)30(4)
InchiKey: FOPCRYWVFXJPNH-UHFFFAOYSA-N
Formula: C32H64O5Si4
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 641.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	11.066		Crippen Method
rinsol	2772.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563329&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/123-203-9/3-4-Dihydroxymandelic-acid-TBDMS.pdf>

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