

3-Hydroxymandelic acid, O,O-bis(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl
silyl tert-butyl dimethylsilyl ester, 3-pyrrolo[tert-butyl(dimethyl)silyl]oxymorphophen
3-Hydroxymandelic acid, 3tbdms derivative

Inchi: InChI=1S/C26H50O4Si3/c1-24(2,3)31(10,11)28-21-18-16-17-20(19-21)22(29-32(12,13)2
InchiKey: IUYHMCKPQSHYDV-UHFFFAOYSA-N
Formula: C26H50O4Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C(O[Si](C)(C)C(C)(C)C)c1cccc(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 510.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	8.682		Crippen Method
rinpol	2343.50		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=U332761&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
rinpol: Non-polar retention indices

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