

3,4-Dihydroxybenzylamine, N-isoBOC, O-TBDMS

Inchi:	InChI=1S/C24H45NO4Si2/c1-18(2)17-27-22(26)25-16-19-13-14-20(28-30(9,10)23(3,4)5)
InchiKey:	ADJJDUGHPCMVNR-UHFFFAOYSA-N
Formula:	C24H45NO4Si2
SMILES:	CC(C)COC(=O)NCc1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	467.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	7.337		Crippen Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392360&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

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<https://www.cheméo.com/cid/114-922-1/3-4-Dihydroxybenzylamine-N-isoBOC-O-TBDMS.pdf>

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