

8'-HOCH2-ABA, Me-TMS

Other names:	8'-Hydroxymethyl-ABA, Me-TMS
Inchi:	InChI=1S/C22H38O5Si2/c1-17(13-20(24)25-4)11-12-22(27-29(8,9)10)18(2)14-19(23)15-
InchiKey:	VXZSFPICJXXBKL-FZABIRJSSA-N
Formula:	C22H38O5Si2
SMILES:	<chem>COC(=O)C=C(C)C=CC1(O[Si](C)(C)C)C(C)=CC(=O)CC1(C)CO[Si](C)(C)C</chem>
Mol. weight [g/mol]:	438.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.78		Crippen Method
logp	5.029		Crippen Method
rinpol	2272.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2272.00		NIST Webbook
rinpol	2270.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536877&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

Latest version available from:

<https://www.chemeo.com/cid/59-412-9/8-HOCH2-ABA-Me-TMS.pdf>

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