Benzeneacetic acid, «alpha»-[[(trimethylsilyl)oxy]methyl]-, 9-methyl-3-oxa-9-azatricyclo[3.3.1.0(2,4)]non-7-yl ester, [7(S)-(1«alpha»,2«beta»,4«beta»,5«alpha»,7«beta»

Other names: Scopolamine hydrobromide, trimethylsilyl ether
Inchi: InChI=1S/C20H29NO4Si/c1-21-16-10-14(11-17(21)19-18(16)25-19)24-20(22)15(12-23-2
Inchikey: KYAGWQUTVDHVGQ-UHFFFAOYSA-N
Formula: C20H29NO4Si
SMILES: CN1C2CC(OC(=O)C(CO[Si](C)(C)C)c3ccccc3)CC1C1OC12
Mol. weight [g/mol]: 375.53
CAS: 55373-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	2.777		Crippen Method
rinpol	2400.80		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55373836&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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