Benzeneacetic acid, «alpha»-[[(trimethylsilyl)oxy]methyl]-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, endo-(.+/-.)-

Other names:	Benzeneacetic acid, «alpha»-[[(trimethylsilyl)oxy]methyl]-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, endo-(.+/-.)-
	Monotrimethylsilyl-derivative of Atropine
	Atropine TMS derivative
	Atropine, o-trimethylsilyl-
	Atropine, trimethylsilyl ether
	8-Methyl-8-azabicyclo[3.2.1]oct-3-yl 2-phenyl-3-[(trimethylsilyl)oxy]propanoate
Inchi:	InChI=1S/C20H31NO3Si/c1-21-16-10-11-17(21)13-18(12-16)24-20(22)19(14-23-25(2,3)4
InchiKey:	ZYDHKQGYYADXRL-UHFFFAOYSA-N
Formula:	C20H31NO3Si
SMILES:	CN1C2CCC1CC(OC(=O)C(CO[Si](C)(C)C)c1ccccc1)C2
Mol. weight [g/mol]:	361.55
CAS:	55334-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	3.790		Crippen Method
rinpol	2298.60		NIST Webbook
rinpol	2298.60		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334037&Units=SI

Legend

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