

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)-

InchiKey: ZYDHKQGYADXRLL-UHFFFAOYSA-N

Formula: C20H31NO3Si

SMILES: CN1C2CCC1CC(OC(=O)C(CO[Si](C)(C)C)c1cccc1)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/ci9903071>

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

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