2-Butenoic acid, 2-methyl-,8-methyl-6-(1-oxopropoxy)-8-azabicyclo ester, [1R-[1«alpha»,3«beta»(E),5«alpha»,6«alpha»]]-

Othernames: 3-Tigloyloxy-6-propionyloxytropane
Inchi: InChI=1S/C16H25NO4/c1-5-10(3)16(19)20-12-7-11-8-14(21-15(18)6-2)13(9-12)17(11)4/h
InchiKey: [illegible]
Formula: C16H25NO4
SMILES: CC=C(C)C(=O)OC1CC2CC(OC(=O)CC)C(C1)N2C
Mol. weight [g/mol]: 295.37
CAS: 54354-59-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.053		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54354595&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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