6-Acetylglyoxy-3-tigloyltropine

Inchi: InChI=1S/C17H25NO6/c1-5-10(2)17(21)23-13-6-12-7-15(14(8-13)18(12)4)24-16(20)9-22
InchiKey: PSIIWCWCSQBEJC-QSBADXEOSA-N
Formula: C17H25NO6
SMILES: CC=C(C)C(=O)OC1CC2CC(OC(=O)COC(C)=O)C(C1)N2C
Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	1.206		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R585290&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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