3«alpha»-Tigloyloxy-6«beta»-isovaleryloxy-7«beta

Inchi: InChI=1S/C18H29NO5/c1-6-11(4)18(22)23-12-8-13-16(21)17(14(9-12)19(13)5)24-15(20)
InchiKey: NQACTVWQBJPZMD-DDMBWBHOSA-N
Formula: C18H29NO5
SMILES: CC=C(C)C(=O)OC1CC2C(O)C(OC(=O)CC(C)C)C(C1)N2C
Mol. weight [g/mol]: 339.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.660		Crippen Method
mcvol	269.190	ml/mol	McGowan Method
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R421453&Units=SI

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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