13-Tigloyloxy-17-oxolupanine

Inchi: InChI=1S/C20H28N2O4/c1-3-12(2)20(25)26-14-7-8-21-17(10-14)13-9-15(19(21)24)16-5-
InchiKey: HUDZBAALYALAER-KGVSQERTSA-N
Formula: C20H28N2O4
SMILES: CC=C(C)C(=O)OC1CCN2C(=O)C3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 360.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	1.886		Crippen Method
mcvol	275.460	ml/mol	McGowan Method
rinpol	2971.00		NIST Webbook
rinpol	2905.00		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=R205395&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.