

3-Tigloyloxy-6-propionyloxy-7-hydroxytropone

Inchi: InChI=1S/C16H25NO5/c1-5-9(3)16(20)21-10-7-11-14(19)15(22-13(18)6-2)12(8-10)17(11)
InchiKey: HGOLJZZEGFBRMR-WEVVVXLNSA-N
Formula: C16H25NO5
SMILES: CC=C(C)C(=O)OC1CC2C(O)C(OC(=O)CC)C(C1)N2C
Mol. weight [g/mol]: 311.37
CAS: 872205-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	1.023		Crippen Method
mcvol	241.010	ml/mol	McGowan Method
rinpol	1985.80		NIST Webbook
rinpol	1985.80		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C872205339&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

Latest version available from:

<https://www.chemeo.com/cid/82-441-1/3-Tigloyloxy-6-propionyloxy-7-hydroxytropone.pdf>

Generated by Cheméo on 2024-04-24 04:56:22.148781991 +0000 UTC m=+16223831.069359302.

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