

6-Tigloyloxyhyoscyamine

Inchi:	InChI=1S/C22H29NO5/c1-4-14(2)21(25)28-20-11-16-10-17(12-19(20)23(16)3)27-22(26)
InchiKey:	OPGJHCLCUNWOSH-HUIKIPCCSA-N
Formula:	C22H29NO5
SMILES:	CC=C(C)C(=O)OC1CC2CC(OC(=O)C(CO)c3ccccc3)CC1N2C
Mol. weight [g/mol]:	387.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	2.419		Crippen Method
mcvol	301.790	ml/mol	McGowan Method
rinpola	2649.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421740&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/12-193-4/6-Tigloyloxyhyoscyamine.pdf>

Generated by Cheméo on 2024-04-27 15:25:59.311390801 +0000 UTC m=+16520808.231968117.

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