

Tigloidine

Other names:	3«beta»-Tigloyloxytropane
Inchi:	InChI=1S/C13H21NO2/c1-4-5-13(15)16-12-8-10-6-7-11(9(12)2)14(10)3/h4-5,9-12H,6-8H
InchiKey:	UCFGSCGYIQQNQV-FYURHTHTOSA-N
Formula:	C13H21NO2
SMILES:	CC=CC(=O)OC1CC2CCC(C1C)N2C
Mol. weight [g/mol]:	223.31
CAS:	495-83-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	1.977		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpola	1904.10		NIST Webbook

Sources

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=C495830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/41-893-5/Tigloidine.pdf>

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