

# 4,8-Secosenecionan-8,11,16-trione, 15,20-dihydro-12-(acetyloxy)-20-chloro-15-hydroxy

Other names:	Doronine
Inchi:	4,8-Secosenecionan-8,11,16-trione, 12-(acetyloxy)-20-chloro-15,20-dihydro-15-hydroxy-4-methyl-, (15 $\alpha$ ), 20R) InChI=1S/C21H30ClNO8/c1-12-10-21(28,13(2)22)19(27)30-16-7-9-23(5)8-6-13(17(16)25
InchiKey:	VGRSISYREBBIAL-UUASQNMZSA-N
Formula:	C21H30ClNO8
SMILES:	CC(=O)OC1(C)C(=O)OCC2=CCN(C)CCC(OC(=O)C(O)(C(C)Cl)CC1C)C2=O
Mol. weight [g/mol]:	459.92
CAS:	60367-00-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	0.992		Crippen Method
mcvol	332.710	ml/mol	McGowan Method
rinpol	2849.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C60367002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60367002&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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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