

Monocrotaline

Other names:

20-Norcrotalanan-11,15-dione, 14,19-dihydro-12,13-dihydroxy-,
(13«alpha»,14«alpha»)-
Monocrotalin

(2,3,4-gh)pyrrolizine-2,6(3H)-dione,
(4,5,8,10,12,13,13a,13b)-octahydro-4,5-dihydroxy-3,4,5-trimethyl-2H-(1,6)dioxacycloundecino
A 6080

NCI-C56462

NSC 28693

Retronecine cyclic 2,3-dihydroxy-2,3,4-trimethylglutarate

12«beta»,13«beta»-Dihydroxy-12«alpha»,13«alpha»,14«alpha»-trimethylcrotal-1-enine

14,19-Dihydro-12,13-dihydroxy(13«alpha»,14«alpha»)-20-norcrotalanan-11,15-dione

Crotaline

(13-«alpha»,14-«alpha»)-14,19-Dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dione

2H-[1,6]Dioxacycloundecino[2,3,4-gh]pyrrolizine, 20-norcrotalanan-11,15-dione

deriv.
2H-[1,6]Dioxacycloundecino[2,3,4-gh]pyrrolizine-2,6(3H)-dione,

4,5,8,10,12,13,13a,13b-octahydro-4,5-dihydroxy-3,4,5-trimethyl-
InChI=1S/C16H23NO6/c1-9-13(18)23-11-5-7-17-6-4-10(12(11)17)8-22-14(19)16(3,21)15
(3R,4R,5R,13aR,13bR)-

Inchi:**InchiKey:**

QVCMHGGNRFRMAD-UHFFFAOYSA-N

Formula:

C16H23NO6

SMILES:

CC1C(=O)OC2CCN3CC=C(COC(=O)C(C)(O)C1(C)O)C23

Mol. weight [g/mol]:

325.36

CAS:

315-22-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	-0.393		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
rinpol	2270.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2268.00		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=C315220&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
rinpol:	Non-polar retention indices

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