

Levallorphan

Other names:

Morphinan-3-ol, 17-(2-propenyl)-
Morphinan-3-ol, 17-allyl-
L-N-allyl-3-hydroxymorphinan
N-Allyl-3-hydroxymorphinan
17-Allylmorphinan-3-ol
(-)-3-Hydroxy-N-allylmorphinan
levo-3-Hydroxy-N-allyl morphinan
Morphinan, 17-allyl-3-hydroxy-
Naloxiphan
RO-1-7700

Inchi:

InChI=1S/C19H25NO/c1-2-10-20-11-9-19-8-4-3-5-16(19)18(20)12-14-6-7-15(21)13-17(1)

InchiKey:

OZYUPQUCAUTOBP-UHFFFAOYSA-N

Formula:

C19H25NO

SMILES:

C=CCN1CCC23CCCCC2C1Cc1ccc(O)cc13

Mol. weight [g/mol]:

283.41

CAS:

152-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.637		Crippen Method
mcvol	233.780	ml/mol	McGowan Method
rinpol	2360.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2306.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2306.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2340.00		NIST Webbook
ripol	3665.00		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=C152023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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