

Nalorphine

Other names:	Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-(2-propenyl)-, (5«alpha»,6«alpha»)- Morphinan-3,6«alpha»-diol, 17-allyl-7,8-didehydro-4,5«alpha»-epoxy- Allorphine Anarcon Anthorphine Antorfin Antorphin Antorphine Lethidrone Letidron N-Allylnormorphine Nallin Nalline Nalorphin Norfin NANM Acetorfin N-Allyl-7,8-dehydro-4,5-epoxy-3,6-dihydroxymorphinan N-Allyl-N-desmethylnormorphine Nalorfina Nalorphinium Normorphine, N-allyl- 17-Allyl-7,8-didehydro-4,5«alpha»-epoxymorphinan-3,6«alpha»-diol Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-(2-propen-1-yl)-, (5«alpha»,6«alpha»)- InChI=1S/C19H21NO3/c1-2-8-20-9-7-19-12-4-6-15(22)18(19)23-17-14(21)5-3-11(16(17))
Inchi:	
InchiKey:	UIQMVEYFGZJHCZ-UHFFFAOYSA-N
Formula:	C19H21NO3
SMILES:	C=CCN1CCC23c4c5ccc(O)c4OC2C(O)C=CC3C1C5
Mol. weight [g/mol]:	311.37
CAS:	62-67-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	1.754		Crippen Method
mcvol	230.360	ml/mol	McGowan Method

rinpol	2577.00	NIST Webbook
rinpol	2570.00	NIST Webbook
rinpol	2678.20	NIST Webbook
rinpol	2580.00	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=C62679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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