

Nalmefene

Other names:

Morphinan-3,14-diol, 17-(cyclopropylmethyl)-4,5-epoxy-6-methylene-, (5«alpha»)-
17-(Cyclopropylmethyl)-4,5«alpha»-epoxy-6-methylenemorphinan-3,14-diol

Nalmetrene

JF-1

ORF-11676

Inchi:

InChI=1S/C21H25NO3/c1-12-6-7-21(24)16-10-14-4-5-15(23)18-17(14)20(21,19(12)25-18

InchiKey:

WJBLNOPPDWQMCH-UHFFFAOYSA-N

Formula:

C₂₁H₂₅NO₃

SMILES:

C=C1CCC2(O)C3Cc4ccc(O)c5c4C2(CCN3CC2CC2)C1O5

Mol. weight [g/mol]:

339.43

CAS:

55096-26-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	2.512		Crippen Method
mcvol	251.980	ml/mol	McGowan Method
rinpol	2797.60		NIST Webbook
rinpol	2797.60		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55096269&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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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