

7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazepine-2-hydroxy-,

Other names:

Nuttaline

Nuttaline

[2S-(2«alpha»,7«alpha»,7a«beta»,14«alpha»,14a«alpha»)]-S(=O)(=O)C1=CC=C(C=C1)N2C=CC(=O)N2C3=CC=CC=C3

InchiKey: GIQKWLHFWBBSSV-UHFFFAOYSA-N

Formula: C₁₅H₂₄N₂O₂

SMILES: O=C1CC(O)CC2C3CC(CN12)C1CCCCN1C3

Mol. weight [g/mol]: 264.36

CAS: 23360-87-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	0.842		Crippen Method
mcvol	206.170	ml/mol	McGowan Method
rinpol	2255.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23360874&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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