

Lincomycin

Other names:

D-erythro-«alpha»-D-galacto-Octopyranoside, methyl
6,8-dideoxy-6-[[[(1-methyl-4-propyl-2-pyrrolidinyl)carbonyl]amino]-1-thio-,
D-erythro-D-galacto-Octopyranoside, methyl
2S-trans)-
6,8-dideoxy-6-(1-methyl-4-propyl-L-2-pyrrolidinecarboxamido)-1-thio-, trans-
«alpha»-
Lincocin
Lincocine
Lincolcina
Lincomyocin
U 10,149A
Lincolnensin
Lincomycine
NSC-70731
U-10149
Methyl
6,8-dideoxy-6-trans-(1-methyl-4-propyl-L-2-pyrrolidinecarboxamido)-1-thio-D-erythro-«alp
Jemycin
Lincomycin A

Inchi:

InChI=1S/C18H34N2O6S/c1-5-6-10-7-11(20(3)8-10)17(25)19-12(9(2)21)16-14(23)13(22)

InchiKey:

OJMMVQQUTAEWLP-UHFFFAOYSA-N

Formula:

C18H34N2O6S

SMILES:

CCCC1CC(C(=O)NC(C(C)O)C2OC(SC)C(O)C(O)C2O)N(C)C1

Mol. weight [g/mol]:

406.54

CAS:

154-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	-0.857		Crippen Method
mcvol	309.990	ml/mol	McGowan Method

Sources

Crippen Method:

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

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=C154212&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/18-744-6/Lincomycin.pdf>

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