Tetracycline

Other names:

(-)-Tetracycline

(4S,4aS,5aS,12aS)-4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pe

(4S,4aS,5aS,6S,12aS)-4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a

2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-

2-Naphthacenecarboxamide, (4S,4aS,5aS,6S,12aS)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-

2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-

2-Naphthacenecarboxamide, [4S-(4«alpha», 4a«alpha», 5a«alpha», 6«beta», 12a«alpha»)]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-

2-Naphthacenecarboxamide, [4S-(4Â«alphaÂ», 4aÂ«alphaÂ», 5aÂ«alphaÂ», 6Â«betaÂ», 12aÂ«alphaÂ»)]-4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl

[4S-(4«alpha», 4a«alpha», 5a«alpha», 6«beta», 12a«alpha»)]-4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl

[4S-(4Â«alphaÂ», 4aÂ«alphaÂ», 5aÂ«alphaÂ», 6Â«betaÂ», 12aÂ«alphaÂ»)]-4-(Dimethylamino)-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-1,4,4a,5,5a,6,11,12a

[4S-(4«alpha», 4a«alpha», 5a«alpha», 6«beta», 12a«alpha»)]-4-(Dimethylamino)-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-1,4,4a,5,5a,6,11,12a

Abramycin

[4S-(4Â«alphaÂ»,4aÂ«alphaÂ»,5aÂ«alphaÂ»,6Â«betaÂ»,12aÂ«alphaÂ»)]-

Abricycline

Achromycin

Acromicina

Agromicina

Ambramicina

Ambramycin

Amycin

Bio-tetra

Biocycline

Bristaciclin «alpha»

Bristaciclin Â«alphaÂ»

Bristaciclina

Cefracycline

Cefracycline suspension

Centet (base)

Ciclibion

Copharlan

Criseociclina

Cyclomycin

Cytome

Democracin

Deschlorobiomycin

Dispatetrin

Enterocycline

Hostacyclin

Ibicyn

Lemtrex (base)

Lexacycline

Limecycline
Liquamycin
Liquamycin, veterinary
Medocycline
Mericycline
Micycline
Neocycline
Omegamycin
Orlycycline
Panmycin
Piracaps (base)
Polycycline
Polycycline, antibiotic
Purocyclina
Resteclin
Robitet
Roviciclina
SK-Tetracycline
Sanclomycine
Sigmamycin
Steclin
T-125
Tetra-Co
Tetra-Proter
Tetrabon
Tetracycline I
Tetracycline II
Tetracyn
Tetradecin
Tetrafil
Tetraseptine
Tetraverine
Tsiklomitsin
Veracin
Vetacyclinum
Vetquamycin-324 (free base)

Inchi: InChI=1S/C22H24N2O8/c1-21(31)8-5-4-6-11(25)12(8)16(26)13-9(21)7-10-15(24(2)3)17(

InchiKey: OFVLGDICTFRJMM-UHFFFAOYSA-N

Formula: C22H24N2O8

SMILES: CN(C)C1C(O)=C(C(N)=O)C(=O)C2(O)C(O)=C3C(=O)c4c(O)cccc4C(C)(O)C3CC12

Mol. weight [g/mol]: 444.43

CAS: 60-54-8

Physical Properties

Property code	Value	Unit	Source
gf	-520.68	kJ/mol	Joback Method
hf	-1085.84	kJ/mol	Joback Method
hfus	55.90	kJ/mol	Joback Method
hvap	175.73	kJ/mol	Joback Method
log10ws	-2.44		Aqueous Solubility Prediction Method
logp	-0.214		Crippen Method
mcvol	309.920	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	1500.65	K	Joback Method
tc	1927.79	K	Joback Method
tf	323.65	K	Aqueous Solubility Prediction Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1614.66	J/mol×K	1500.65	Joback Method
cpg	1742.02	J/mol×K	1571.84	Joback Method
cpg	1888.30	J/mol×K	1643.03	Joback Method
cpg	2055.42	J/mol×K	1714.22	Joback Method
cpg	2245.34	J/mol×K	1785.41	Joback Method
cpg	2459.98	J/mol×K	1856.60	Joback Method
cpg	2701.27	J/mol×K	1927.79	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60548&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume