RIBOFLAVINE

Other names:

6,7-Dimethyl-9-D-ribitylisoalloxazine
7,8-Dimethyl-10-(d-ribo-2,3,4,5-tetrahydroxypentyl)isoalloxazine
7,8-Dimethyl-10-ribitylisoalloxazine
Aqua-Flave
Beflavin
Beflavine
Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8-dimethyl-10-(D-ribo-2,3,4,5-tetrahydroxypentyl)-
D-Ribitol, 1-deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl)-
Dermadram
Fiboflavin
Flavaxin
Flavin BB
Flaxain
Hyflavin
Hyre
Isoalloxazine, 7,8-dimethyl-10-(D-ribo-2,3,4,5-tetrahydroxypentyl)-
Isoalloxazine, 7,8-dimethyl-10-D-ribityl-
Lactobene
Lactoflavin
Lactoflavine
Lactoflavine, zinvit-g
NSC 33298
Ovoflavin
Ribipca
Ribocrisina
Riboderm
Ribosyn
Ribotone
Ribovel
Russupteridine Yellow III
Vitaflavine
Vitamin B2
Vitamin Bi
Vitamin G
Vitasan B2
riboflavin

Inchi: InChI=1S/C17H20N4O6/c1-7-3-9-10(4-8(7)2)21(5-11(23)14(25)12(24)6-22)15-13(18-9)1

InchiKey: AUNGANRZJHBGPY-UHFFFAOYSA-N

Formula: C17H20N4O6

SMILES: Cc1cc2nc3c(=O)[nH]c(=O)nc-3n(CC(O)C(O)C(O)CO)c2cc1C

Mol. weight [g/mol]: 376.37

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-3.68		Aqueous Solubility Prediction Method
log10ws	-3.69		Estimated Solubility Method
logp	-2.205		Crippen Method
mcvol	262.850	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83885&Units=SI

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

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

Cheméo Relay (1.0):

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume