

Riboflavin, 2',3',4',5'-tetrabutanoate

Other names:

7,8-Dimethyl-10-(d-ribo-2,3,4,5-tetrahydroxypentyl)isoalloxazine
2,3,4,5-tetrabutryate
Bituvitan
Eyekas
Hibon
Lacflavin
Riboflavin 2,3,4,5-tetrabutryate
Ribolact
Viras
Wakaflavin L
Riboflavin tetrabutryate

Inchi:

InChI=1S/C33H44N4O10/c1-7-11-25(38)44-18-24(46-27(40)13-9-3)30(47-28(41)14-10-4

InchiKey:

MJNIIWUJSIGSWKK-UHFFFAOYSA-N

Formula:

C33H44N4O10

SMILES:

CCCC(=O)OCC(OC(=O)CCC)C(OC(=O)CCC)C(Cn1c2nc(=O)[nH]c(=O)c-2nc2cc(C)c(C)

Mol. weight [g/mol]:

656.72

CAS:

752-56-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.84		Crippen Method
logp	3.199		Crippen Method
mvol	494.570	ml/mol	McGowan Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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=C752567&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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