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

Other names:	7,8-Dimethyl-10-(d-ribo-2,3,4,5-tetrahydroxypentyl)isoalloxazine 2,3,4,5-tetrabutyrate Bituvitan Eyekas Hibon Lacflavin Riboflavin 2,3,4,5-tetrabutyrate Ribolact Viras Wakaflavin L Riboflavin tetrabutyrate
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:	MJNIWUJSIGSWKK-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
mcvol	494.570	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=C752567&Units=SI

Legend

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