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

Other names:	Riboflavin tetraacetate
	Riboflavine tetraacetate
	Riboflavine, 2',3',4',5'-tetraacetate
	Tetra-O-acetylriboflavine
	Tetraacetylriboflavin
	Tetraacetylriboflavine
	Vitamin B2 tetraacetate
	2',3',4',5'-Tetra-O-acetylriboflavin
Inchi:	InChI=1S/C25H28N4O10/c1-11-7-17-18(8-12(11)2)29(23-21(26-17)24(34)28-25(35)27-2
InchiKey:	VKVDYPHLGLIXAG-UHFFFAOYSA-N
Formula:	C25H28N4O10
SMILES:	CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(Cn1c2nc(=O)[nH]c(=O)c-2nc2cc(C)c(C)cc21)OC(
Mol. weight [g/mol]:	544.51
CAS:	752-13-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	0.078		Crippen Method
mcvol	381.850	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C752136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume