

# Riboflavin, 2',3',4',5'-tetrapropanoate

<b>Other names:</b>	Riboflavine, 2',3',4',5'-tetrapropionate Riboflavin tetrapropionate Riboflavine tetrapropionate Riboflavine, 2',3',4',5'-tetrapropanoate Vitamin B2 tetrapropionate
<b>Inchi:</b>	InChI=1S/C29H36N4O10/c1-7-21(34)40-14-20(42-23(36)9-3)26(43-24(37)10-4)19(41-22
<b>InchiKey:</b>	SHKSLTFASOOBHE-UHFFFAOYSA-N
<b>Formula:</b>	C29H36N4O10
<b>SMILES:</b>	CCC(=O)OCC(OC(=O)CC)C(OC(=O)CC)C(Cn1c2nc(=O)nc(O)c-2nc2cc(C)c(C)cc21)OC
<b>Mol. weight [g/mol]:</b>	600.62
<b>CAS:</b>	7652-80-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.84		Crippen Method
logp	2.532		Crippen Method
mcvol	438.210	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7652804&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7652804&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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