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

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

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=C7652804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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