

Nicofuranose

Other names:	«beta»-D-Fructofuranose, 1,3,4,6-tetra-3-pyridinecarboxylate D-Fructofuranose 1,3,4,6-tetranicotinate Bradilan Vasperdil
Inchi:	InChI=1S/C30H24N4O10/c35-26(19-5-1-9-31-13-19)40-17-23-24(42-28(37)21-7-3-11-33
InchiKey:	FUWFSXZKBMCSKF-UHFFFAOYSA-N
Formula:	C30H24N4O10
SMILES:	O=C(OCC1OC(O)(COC(=O)c2ccnc2)C(OC(=O)c2ccnc2)C1OC(=O)c1ccnc1)c1ccnc1
Mol. weight [g/mol]:	600.53
CAS:	15351-13-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	1.819		Crippen Method
mcvol	409.080	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15351130&Units=SI
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

Legend

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

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