

1H-pyrazolo[3,4-d]pyrimidine, 4-(methylthio)-1-beta-d-ribofuranosyl-, 2,3,5'-tribenzoate

InChI: InChI=1S/C32H26N4O7S/c1-44-28-23-17-35-36(27(23)33-19-34-28)29-26(43-32(39)22-23)31-30-25-24-21-20-18-16-15-14-13-12-11-10-9-8-7-6-5-4-3-2-1/s1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100

InChIKey: YHAI0CH0FVWVOS-UHFFFAOYSA-N

Formula: C₃₂H₂₆N₄O₇S

SMILES: CSc1ncnc2c1cnn2C1OC(COC(=O)c2ccccc2)C(OC(=O)c2ccccc2)C1OC(=O)c1ccccc1

Mol. weight [g/mol]: 610.64

CAS: 106488-32-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.03		Crippen Method
logp	4.754		Crippen Method
mcvol	425.140	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C106488328&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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