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)22-1
InchiKey: YHAIOCHOFVWVOS-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: 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
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