

9H-purine-6(1h)-thione, 2-amino-9-beta-d-ribofuranosyl-, 2,3,5'-tribenzoate

InChI: InChI=1S/C31H25N5O7S/c32-31-34-25-22(26(44)35-31)33-17-36(25)27-24(43-30(39)20
InChIKey: RSBGANDZBGTUFE-UHFFFAOYSA-N

Formula: C31H25N5O7S
SMILES: Nc1nc2c(ncn2C2OC(COC(=O)c3ccccc3)C(OC(=O)c3ccccc3)C2OC(=O)c2ccccc2)c(=S)[
Mol. weight [g/mol]: 611.62
CAS: 88010-92-8

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.22 | | Crippen Method |
| logp | 3.795 | | Crippen Method |
| mcvol | 421.030 | ml/mol | McGowan Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C88010928&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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