Adenosine, 2'-deoxy-N-(trifluoroacetyl)-, 3',5'-bis(trifluoroacetate)

Other names: N6,O-3',5'-Tris(trifluoroacetyl)-2'-deoxyadenosine
2'-Deoxyadenosine, N,O,O'-tris(trifluoroacetyl)-

Inchi: InChI=1S/C16H10F9N5O6/c17-14(18,19)11(31)29-9-8-10(27-3-26-9)30(4-28-8)7-1-5(36-

InchiKey: BNSWSPZQTNYLGI-UHFFFAOYSA-N

Formula: C16H10F9N5O6

SMILES: O=C(Nc1ncnc2c1ncn2C1CC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)O1)C(F)(F)F

Mol. weight [g/mol]: 539.27

CAS: 35170-10-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.34		Crippen Method
logp	2.194		Crippen Method
mcvol	274.670	ml/mol	McGowan Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook

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=C35170106&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

rinpol: Non-polar retention indices