5'-S-Methyl-5'-thioadenosine, O,O'-bis(trifluoroacetyl)-

Inchi: InChI=1S/C15H13F6N5O5S/c1-32-2-5-7(30-12(27)14(16,17)18)8(31-13(28)15(19,20)21)

InchiKey: XIKNMXIIAMFOHZ-UHFFFAOYSA-N

Formula: C15H13F6N5O5S

SMILES: CSCC1OC(n2cnc3c(N)ncnc32)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F

Mol. weight [g/mol]: 489.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	1.617		Crippen Method
mcvol	270.050	ml/mol	McGowan Method
rinpol	2341.80		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380308&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices