

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: XIKNMXIAMFOHZ-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

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