

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

Other names:	N4,O3',O5'-Tris(trifluoroacetyl)-2'-deoxycytidine 2'-Deoxycytidine, N,O,O'-tris(trifluoroacetyl)-
Inchi:	InChI=1S/C15H10F9N3O7/c16-13(17,18)9(28)25-7-1-2-27(12(31)26-7)8-3-5(34-11(30)15)
InchiKey:	FSRWMUNYVVLXME-UHFFFAOYSA-N
Formula:	C15H10F9N3O7
SMILES:	O=C(Nc1ccn(C2CC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)O2)c(=O)n1)C(F)(F)F
Mol. weight [g/mol]:	515.24
CAS:	35221-99-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	1.611		Crippen Method
mcvol	261.650	ml/mol	McGowan Method
rinpol	2176.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C35221999&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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