

Uridine, 2'-deoxy-, 3',5'-bis(trifluoroacetate)

Other names: 2'-Deoxyuridine, O,O'-bis(trifluoroacetate)-
Inchi: InChI=1S/C13H10F6N2O7/c14-12(15,16)9(23)26-4-6-5(28-10(24)13(17,18)19)3-8(27-6)2
InchiKey: HNOQBJVTAZRPRU-UHFFFAOYSA-N
Formula: C13H10F6N2O7
SMILES: O=C(OCC1OC(n2ccc(=O)[nH]c2=O)CC1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 420.22
CAS: 35170-15-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	-0.078		Crippen Method
mcvol	222.480	ml/mol	McGowan Method
rinpola	2022.60		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=C35170151&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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