PUBCHEM > REMDESIVIR > COMPUTED PROPERTIES

CID 121304016

Remdesivir

Computed Properties



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Property NameProperty ValueReferenceMolecular Weight602.6 g/molComputed by PubChem 2.1 (PubChem release 2019.06.18)XLogP3-AA1.9Computed by XLogP3 3.0 (PubChem release 2019.06.18)Hydrogen Bond Donor Count4Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)Hydrogen Bond Acceptor Count13Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)Rotatable Bond Count14Computed by PubChem 2.1 (PubChem release 2019.06.18)Exact Mass602.225399 g/molComputed by PubChem 2.1 (PubChem release 2019.06.18)Monoisotopic Mass602.225399 g/molComputed by PubChem 2.1 (PubChem release 2019.06.18)Topological Polar Surface Area204 ŲComputed by PubChem 2.1 (PubChem release 2019.06.18)Heavy Atom Count42Computed by PubChemFormal Charge0Computed by PubChemGomplexity1010Computed by PubChemBotope Atom Count0Computed by PubChemDefined Atom Stereocenter Count0Computed by PubChemUndefined Atom Stereocenter Count0Computed by PubChemDefined Bond Stereocenter Count0Computed by PubChemUndefined Bond Stereocenter Count0Computed by PubChemUndefined Bond Stereocenter Count0Computed by PubChemComputed by PubChemComputed by PubChemComputed by PubChemComputed by PubChemCompound Is Canonicalized1Computed by PubChem			
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Hydrogen Bond Acceptor Count 13 Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) Rotatable Bond Count 14 Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) Exact Mass 602.225399 g/mol Computed by PubChem 2.1 (PubChem release 2019.06.18) Monoisotopic Mass 602.225399 g/mol Computed by PubChem 2.1 (PubChem release 2019.06.18) Topological Polar Surface Area 204 Ų Computed by PubChem 2.1 (PubChem release 2019.06.18) Heavy Atom Count 42 Computed by PubChem Formal Charge 0 Computed by PubChem Complexity 1010 Computed by PubChem Defined Atom Stereocenter Count 0 Computed by PubChem Defined Atom Stereocenter Count 0 Computed by PubChem Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem	XLogP3-AA	1.9	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
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Topological Polar Surface Area 204 Ų Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) Heavy Atom Count 42 Computed by PubChem Formal Charge 0 Computed by PubChem Complexity 1010 Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) Isotope Atom Count 0 Computed by PubChem Defined Atom Stereocenter Count 6 Computed by PubChem Undefined Atom Stereocenter Count 0 Computed by PubChem Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem	Exact Mass	602.225399 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Heavy Atom Count 42 Computed by PubChem Formal Charge 0 Computed by PubChem Complexity 1010 Computed by PubChem release 2019.06.18) Isotope Atom Count 0 Computed by PubChem Defined Atom Stereocenter Count 6 Computed by PubChem Undefined Atom Stereocenter Count 0 Computed by PubChem Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem	Monoisotopic Mass	602.225399 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Formal Charge 0 Computed by PubChem Complexity 1010 Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) Isotope Atom Count 0 Computed by PubChem Defined Atom Stereocenter Count 6 Computed by PubChem Undefined Atom Stereocenter Count 0 Computed by PubChem Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem Computed by PubChem Computed by PubChem Computed by PubChem	Topological Polar Surface Area	204 Ų	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
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Isotope Atom Count Defined Atom Stereocenter Count Undefined Atom Stereocenter Count Computed by PubChem	Formal Charge	0	Computed by PubChem
Defined Atom Stereocenter Count 6 Computed by PubChem Undefined Atom Stereocenter Count 0 Computed by PubChem Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem Covalently-Bonded Unit Count 1 Computed by PubChem	Complexity	1010	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Undefined Atom Stereocenter Count 0 Computed by PubChem Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem Covalently-Bonded Unit Count 1 Computed by PubChem	Isotope Atom Count	0	Computed by PubChem
Defined Bond Stereocenter Count 0 Computed by PubChem Undefined Bond Stereocenter Count 0 Computed by PubChem Covalently-Bonded Unit Count 1 Computed by PubChem	Defined Atom Stereocenter Count	6	Computed by PubChem
Undefined Bond Stereocenter Count 0 Computed by PubChem Covalently-Bonded Unit Count 1 Computed by PubChem	Undefined Atom Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count 1 Computed by PubChem	Defined Bond Stereocenter Count	0	Computed by PubChem
	Undefined Bond Stereocenter Count	0	Computed by PubChem
Compound Is Canonicalized Yes Computed by PubChem (release 2019.01.04)	Covalently-Bonded Unit Count	1	Computed by PubChem
	Compound Is Canonicalized	Yes	Computed by PubChem (release 2019.01.04)

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Source: PubChem

URL: https://pubchem.ncbi.nlm.nih.gov

 $\textbf{Description:} \ \mathsf{Data} \ \mathsf{deposited} \ \mathsf{in} \ \mathsf{or} \ \mathsf{computed} \ \mathsf{by} \ \mathsf{PubChem}$

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