Adenosine

Other names:	.beta.-adenosine
	6-Amino-9«beta»-D-ribofuranosyl-9H-purine
	6-Amino-9Â«betaÂ»-D-ribofuranosyl-9H-purine
	6-amino-9.beta.-D-ribofuranosyl-9H-purine
	9-.beta.-D-ribofuranosidoadenine
	9-«beta»-D-Ribofuranosidoadenine
	9-«beta»-D-Ribofuranosyl-9H-purin-6-amine
	9-«beta»-d-Ribofuranosyladenine
	9-Â«betaÂ»-D-Ribofuranosidoadenine
	9-Â«betaÂ»-D-Ribofuranosyl-9H-purin-6-amine
	9-Â«betaÂ»-d-Ribofuranosyladenine
	9H-Purin-6-amine, 9-«beta»-d-ribofuranosyl-
	9H-Purin-6-amine, 9-Â«betaÂ»-d-ribofuranosyl-
	Adenine nucleoside
	Adenine riboside
	Adenocard
	Adenocor
	Adenoscan
	Adenosin
	Boniton
	Myocol
	NSC 7652
	Nucleocardyl
	Sandesin
	USAF CB-10
	adenenine riboside
	«beta»-Adenosine
	«beta»-D-Ribofuranose, 1-(6-amino-9H-purin-9-yl)-1-deoxy-
	«beta»-d-Adenosine
	«beta»-d-Ribofuranoside, adenine-9
	Â«betaÂ»-Adenosine
	Â«betaÂ»-D-Ribofuranose, 1-(6-amino-9H-purin-9-yl)-1-deoxy-
	Â«betaÂ»-d-Adenosine
	Â«betaÂ»-d-Ribofuranoside, adenine-9
Inchi:	InChI=1S/C10H13N5O4/c11-8-5-9(13-2-12-8)15(3-14-5)10-7(18)6(17)4(1-16)19-10/h2-4,
InchiKey:	OIRDTQYFTABQOQ-UHFFFAOYSA-N
Formula:	C10H13N5O4
SMILES:	Nc1ncnc2c1ncn2C1OC(CO)C(O)C1O
Mol. weight [g/mol]:	267.24
CAS:	58-61-7

Physical Properties

Property code	Value	Unit	Source
affp	989.30	kJ/mol	NIST Webbook
basg	956.80	kJ/mol	NIST Webbook
log10ws	-1.70		Aqueous Solubility Prediction Method
logp	-1.980		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
tf	507.90	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The partial molar volumes at T = (288.15 to 313.15) K, and the partial molar heat capacities and expansions at T = 298.15 K of cytidine, uridine, and adenosine in aqueous solution:	https://www.doi.org/10.1016/j.jct.2008.01.020
Volumetric properties of the nucleosides adenosine, cytidine, and uridine in aqueous solutions of N,N-dimethylformamide, N-methyl-2-pyrrolidone, and dimethylsulfoxide and propylene glycol:	https://www.doi.org/10.1016/j.jct.2012.12.028
Equilibrium solubility/dissolution thermodynamics and preferential solvation of adenosine in aqueous solutions of N,N-dimethylformamide, N-methyl-2-pyrrolidone, dimethylsulfoxide and propylene glycol:	https://www.doi.org/10.1016/j.jct.2017.07.023
Partial Molar Isentropic and Isothermal Compressions of the Nucleosides Adenosine, Cytidine, and Uridine in Aqueous Solution at 298.15 K:	https://www.doi.org/10.1021/je101264r

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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