

Inosine

Other names:

1,9-dihydro-9- β -D-ribofuranosyl-6H-purin-6-one
9 β -D-Ribofuranosylhypoxanthine
9 β -D-Ribofuranosylhypoxanthine
Atorel
HXR
Hypoxanthine D-riboside
Hypoxanthine ribonucleoside
Hypoxanthine riboside
Hypoxanthine, 9- β -D-ribofuranosyl-
Hypoxanthine, 9- β -D-ribofuranosyl-
Hypoxanthine-9- β -D-ribofuranoside
Hypoxanthosine
INO 495
Ino
Inosie
NSC 20262
Oxiamin
Panholic-L
Pantholic-L
Ribonosine
Selfer
Trophicardyl
 β -D-Ribofuranoside, hypoxanthine-9
 β -Inosine
 β -D-Ribofuranoside, hypoxanthine-9
 β -Inosine

Inchi:

InChI=1S/C10H12N4O5/c15-1-4-6(16)7(17)10(19-4)14-3-13-5-8(14)11-2-12-9(5)18/h2-4,

InchiKey:

UGQMRVRMYASKQ-DEGSGYPDSA-N

Formula:

C10H12N4O5

SMILES:

OCC1OC(n2cnc3c(O)ncnc32)C(O)C1O

Mol. weight [g/mol]:

268.23

CAS:

58-63-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.23		Aqueous Solubility Prediction Method

log10ws	-1.23		Estimated Solubility Method
logp	-1.857		Crippen Method
mvol	171.250	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	2.60	J/molxK	11.37	Thermochemistry of inosine
cps	5.24	J/molxK	12.40	Thermochemistry of inosine
cps	5.34	J/molxK	13.27	Thermochemistry of inosine
cps	8.00	J/molxK	14.37	Thermochemistry of inosine
cps	8.66	J/molxK	15.72	Thermochemistry of inosine
cps	10.48	J/molxK	17.23	Thermochemistry of inosine
cps	12.67	J/molxK	18.81	Thermochemistry of inosine
cps	15.53	J/molxK	20.54	Thermochemistry of inosine
cps	18.02	J/molxK	22.47	Thermochemistry of inosine
cps	24.46	J/molxK	27.18	Thermochemistry of inosine
cps	27.83	J/molxK	29.58	Thermochemistry of inosine
cps	28.21	J/molxK	29.75	Thermochemistry of inosine
cps	31.55	J/molxK	32.27	Thermochemistry of inosine
cps	32.20	J/molxK	32.59	Thermochemistry of inosine
cps	35.87	J/molxK	35.10	Thermochemistry of inosine
cps	40.23	J/molxK	38.23	Thermochemistry of inosine
cps	44.31	J/molxK	41.70	Thermochemistry of inosine
cps	49.69	J/molxK	45.53	Thermochemistry of inosine
cps	55.90	J/molxK	50.00	Thermochemistry of inosine
cps	63.87	J/molxK	56.53	Thermochemistry of inosine

cps	67.11	J/molxK	59.44	Thermochemistry of inosine
cps	71.10	J/molxK	62.82	Thermochemistry of inosine
cps	75.88	J/molxK	67.13	Thermochemistry of inosine
cps	81.04	J/molxK	71.89	Thermochemistry of inosine
cps	86.11	J/molxK	76.69	Thermochemistry of inosine
cps	91.05	J/molxK	81.53	Thermochemistry of inosine
cps	93.28	J/molxK	83.70	Thermochemistry of inosine
cps	98.01	J/molxK	88.48	Thermochemistry of inosine
cps	102.75	J/molxK	93.41	Thermochemistry of inosine
cps	107.57	J/molxK	98.36	Thermochemistry of inosine
cps	112.18	J/molxK	103.34	Thermochemistry of inosine
cps	116.72	J/molxK	108.27	Thermochemistry of inosine
cps	121.21	J/molxK	113.23	Thermochemistry of inosine
cps	125.64	J/molxK	118.26	Thermochemistry of inosine
cps	130.08	J/molxK	123.30	Thermochemistry of inosine
cps	131.85	J/molxK	125.51	Thermochemistry of inosine
cps	134.43	J/molxK	128.35	Thermochemistry of inosine
cps	136.31	J/molxK	130.57	Thermochemistry of inosine
cps	138.85	J/molxK	133.41	Thermochemistry of inosine
cps	140.70	J/molxK	135.64	Thermochemistry of inosine
cps	144.92	J/molxK	140.71	Thermochemistry of inosine
cps	148.45	J/molxK	145.78	Thermochemistry of inosine
cps	149.33	J/molxK	145.80	Thermochemistry of inosine
cps	152.25	J/molxK	149.37	Thermochemistry of inosine
cps	153.61	J/molxK	150.89	Thermochemistry of inosine
cps	156.35	J/molxK	154.48	Thermochemistry of inosine

cps	160.92	J/molxK	159.58	Thermochemistry of inosine
cps	165.03	J/molxK	164.68	Thermochemistry of inosine
cps	169.62	J/molxK	169.79	Thermochemistry of inosine
cps	173.93	J/molxK	174.90	Thermochemistry of inosine
cps	178.35	J/molxK	180.02	Thermochemistry of inosine
cps	182.52	J/molxK	185.14	Thermochemistry of inosine
cps	187.12	J/molxK	190.27	Thermochemistry of inosine
cps	188.80	J/molxK	192.50	Thermochemistry of inosine
cps	191.39	J/molxK	195.39	Thermochemistry of inosine
cps	192.66	J/molxK	197.62	Thermochemistry of inosine
cps	195.81	J/molxK	200.52	Thermochemistry of inosine
cps	197.62	J/molxK	202.76	Thermochemistry of inosine
cps	202.12	J/molxK	207.88	Thermochemistry of inosine
cps	206.52	J/molxK	213.02	Thermochemistry of inosine
cps	211.07	J/molxK	218.15	Thermochemistry of inosine
cps	215.77	J/molxK	223.29	Thermochemistry of inosine
cps	220.19	J/molxK	228.42	Thermochemistry of inosine
cps	224.73	J/molxK	233.56	Thermochemistry of inosine
cps	229.47	J/molxK	238.70	Thermochemistry of inosine
cps	234.11	J/molxK	243.85	Thermochemistry of inosine
cps	236.41	J/molxK	246.24	Thermochemistry of inosine
cps	238.67	J/molxK	248.99	Thermochemistry of inosine
cps	240.95	J/molxK	251.38	Thermochemistry of inosine
cps	242.17	J/molxK	253.05	Thermochemistry of inosine
cps	245.44	J/molxK	256.52	Thermochemistry of inosine
cps	250.12	J/molxK	261.67	Thermochemistry of inosine

cps	250.43	J/molxK	263.31	Thermochemistry of inosine
cps	254.82	J/molxK	266.82	Thermochemistry of inosine
cps	256.41	J/molxK	268.46	Thermochemistry of inosine
cps	259.52	J/molxK	271.97	Thermochemistry of inosine
cps	260.39	J/molxK	273.61	Thermochemistry of inosine
cps	263.80	J/molxK	277.12	Thermochemistry of inosine
cps	265.31	J/molxK	278.76	Thermochemistry of inosine
cps	269.01	J/molxK	282.28	Thermochemistry of inosine
cps	269.97	J/molxK	283.92	Thermochemistry of inosine
cps	272.96	J/molxK	287.43	Thermochemistry of inosine
cps	274.75	J/molxK	289.07	Thermochemistry of inosine
cps	278.26	J/molxK	292.59	Thermochemistry of inosine
cps	279.92	J/molxK	294.53	Thermochemistry of inosine
cps	282.80	J/molxK	297.74	Thermochemistry of inosine
cps	284.12	J/molxK	299.68	Thermochemistry of inosine
cps	289.53	J/molxK	304.84	Thermochemistry of inosine
cps	294.47	J/molxK	309.99	Thermochemistry of inosine
cps	298.88	J/molxK	315.15	Thermochemistry of inosine
cps	304.00	J/molxK	320.31	Thermochemistry of inosine
cps	308.16	J/molxK	325.47	Thermochemistry of inosine

Sources

Volumetric Properties at High Pressures of the Nucleosides Inosine, 2-Deoxyinosine, and 2-Deoxyguanosine and the Volumetric Properties of Guanosine Derived Using Group Additivity Methods:

NIST Webbook:

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Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Thermochemistry of inosine: <https://www.doi.org/10.1016/j.jct.2005.03.001>
Equilibrium partitioning of drug molecules between aqueous and amino acid ester-based ionic liquids: <https://www.doi.org/10.1016/j.jct.2013.02.011>

Legend

cps: Solid phase heat capacity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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