Thymidine

Other names:
1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1
1-(2-Deoxy-«beta»-D-erythro-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione
1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione
2'-Deoxythymidine
2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-«beta»-D-erythro-pentofuranosyl)-5-methyl-
2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-«beta»-D-ribofuranosyl)-5-methyl-
5-Methyldeoxyuridine
5-Methyldeoxyurindine
5-methyl-2'-deoxyuridine
DThyd
Deoxythymidin
Deoxythymidine
Desoxy-thymidin
NSC 21548
Thymidin
Thymidine, 2'-deoxy-
Thymine-2-Desoxyriboside
Thymine-2-deoxyriboside
Thyminedeoxyriboside
Uridine, 2'-deoxy-5-methyl-
dT
«beta»-D-Ribofuranoside, thymine-1 2-deoxy-

Inchi: InChI=1S/C10H14N2O5/c1-5-3-12(10(16)11-9(5)15)8-2-6(14)7(4-13)17-8/h3,6-8,13-14H
InchiKey: IQFYYKKMVGJFEH-UHFFFAOYSA-N
Formula: C10H14N2O5
SMILES: Cc1cn(C2CC(O)C(CO)O2)c(=O)[nH]c1=O
Mol. weight [g/mol]: 242.23
CAS: 50-89-5

Physical Properties

Property code	Value	Unit	Source
affp	948.30	kJ/mol	NIST Webbook
affp	914.40	kJ/mol	NIST Webbook
basg	915.90	kJ/mol	NIST Webbook
ea	0.40 ± 0.10	eV	NIST Webbook
log10ws	0.28		Crippen Method

logp	-1.996		Crippen Method
mcvol	166.450	ml/mol	McGowan Method
tf	460.15	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	276.70	J/mol×K	298.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	278.84	J/mol×K	303.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	280.97	J/mol×K	308.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	283.12	J/mol×K	313.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	285.25	J/mol×K	318.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	287.40	J/mol×K	323.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	289.53	J/mol×K	328.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	291.68	J/mol×K	333.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine

cps	293.81	J/mol×K	338.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	295.95	J/mol×K	343.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	298.09	J/mol×K	348.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	300.23	J/mol×K	353.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	302.37	J/mol×K	358.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	304.51	J/mol×K	363.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	306.65	J/mol×K	368.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
rhos	1460.00	kg/m3	298.15	Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), thymine(cr), uridine(cr), and xanthine(cr) in H2O(l)

Sources

Volumetric interaction coefficients for some nucleosides in aqueous solution at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2012.12.014
Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine:	https://www.doi.org/10.1021/je800243y
The partial molar heat capacity, expansion, isentropic, and isothermal compressions of thymidine in aqueous solution at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.07.002
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50895&Units=SI
Solvation behavior of some nucleic acid bases and nucleosides in water and in aqueous guanidine hydrochloride solutions: Viscometric, calorimetric and spectroscopic approach:	https://www.doi.org/10.1016/j.jct.2015.11.029

Volumetric studies on nucleic acid bases and nucleosides in aqueous guanidine hydrochloride solutions at T = (288.15 to 318.15) K and at atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2014.10.015
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Homotactic enthalpic pairwise interactions of four deoxynucleosides (dU, dC, dG, dT) in dimethylformamide (DMF) + water mixtures at 298.15 K:	https://www.doi.org/10.1016/j.tca.2012.09.030
Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), thymine(cr), uridine(cr), and xanthine(cr) in H2O(l):	https://www.doi.org/10.1016/j.jct.2004.04.005
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je049551l

Legend

affp:	Proton affinity
basg:	Gas basicity
cps:	Solid phase heat capacity
ea:	Electron affinity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density
tf:	Normal melting (fusion) point