Deoxycytidine

Other names:	2'-Deoxycytidine
	2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-«beta»-D-erythro-pentofuranosyl)-
	2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-Â«betaÂ»-D-erythro-pentofuranosyl)-
	Cytidine, 2'-deoxy-
	Cytosine deoxyribonucleoside
	Cytosine deoxyriboside
	Cytosine, 1-(2-deoxy-«beta»-D-erythro-pentofuranosyl)-
	Cytosine, 1-(2-deoxy-Â«betaÂ»-D-erythro-pentofuranosyl)-
	Deoxyribose cytidine
	Desoxycytidine
	dCYD
Inchi:	InChI=1S/C9H13N3O4/c10-7-1-2-12(9(15)11-7)8-3-5(14)6(4-13)16-8/h1-2,5-6,8,13-14H,3
InchiKey:	CKTSBUTUHBMZGZ-UHFFFAOYSA-N
Formula:	C9H13N3O4
SMILES:	Nc1ccn(C2CC(O)C(CO)O2)c(=O)n1
Mol. weight [g/mol]:	227.22
CAS:	951-77-9

Physical Properties

Property code	Value	Unit	Source
affp	988.40	kJ/mol	NIST Webbook
basg	956.00	kJ/mol	NIST Webbook
ea	0.50 ± 0.10	eV	NIST Webbook
log10ws	-2.14e-03		Crippen Method
logp	-1.534		Crippen Method
mcvol	156.470	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Homotactic enthalpic pairwise interactions of four deoxynucleosides (dC, dG, dA, dT) in dimethylformamide (DMF) + water mixtures at 298.15 K:	https://www.doi.org/10.1016/j.tca.2012.09.030
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C951779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume