

2'-DEOXYGUANOSINE

Other names:	2-Deoxyguanosine 2-amino-9-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-1,9-dihydro-6H-9H-Purin-6-ol, 2-amino-9-(2-deoxy-9-«beta»-D-ribofuranosyl)- Deoxyguanosine Desoxyguanosine Guanine deoxy nucleoside Guanine deoxyriboside Guanine, 9-(2-deoxy-«beta»-D-erythro-pentofuranosyl)- NSC 22837
Inchi:	InChI=1S/C10H13N5O4/c11-10-13-8-7(9(18)14-10)12-3-15(8)6-1-4(17)5(2-16)19-6/h3-6,11,13,15,17,19
InchiKey:	YKBGVTZYEHEMT-UHFFFAOYSA-N
Formula:	C10H13N5O4
SMILES:	Nc1nc(O)c2ncn(C3CC(O)C(CO)O3)c2n1
Mol. weight [g/mol]:	267.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Cheméo Relay (1.0)
logp	-1.245		Crippen Method
mcvol	175.360	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0, beta):	
Volumetric interaction coefficients for some nucleosides in aqueous solution	https://www.doi.org/10.1016/j.jct.2012.12.014
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:	https://www.doi.org/10.1021/jc500458e https://www.chemeo.com/doc/models/crippen_log10ws http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Homotactic enthalpic pairwise interactions of four deoxynucleosides (dG, dC, dA, dU) in dimethylformamide (DMF) + water mixtures at 298.15 K:	https://www.doi.org/10.1016/j.tca.2012.09.030 http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C961079

Legend

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

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