Acyclovir

Other names:	2-Amino-1,9-dihydro-9-((2-hydroxyethoxy)methyl)-6H-purin-6-one 2-Amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one 6H-Purin-6-one, 1,9-dihydro-2-amino-9-((2-hydroxyethoxy)methyl)- 6H-Purin-6-one, 2-amino-1,9-dihydro-9-[(2-hydroxyethoxy)methyl]- 9-(2-Hydroxyethoxymethyl)guanine 9-[(2-hydroxyethoxyl)methyl]guanine ACV Acicloftal Aciclovir Acyclo-V Acycloguanosine BW 248U Cargosil NSC 645011 Poviral Vipral Virorax W-248-U Wellcome-248U Zovirax Zyclir
Inchi:	InChI=1S/C8H11N5O3/c9-8-11-6-5(7(15)12-8)10-3-13(6)4-16-2-1-14/h3,14H,1-2,4H2,(H
InchiKey:	MKUXAQIIEYXACX-UHFFFAOYSA-N
Formula:	C8H11N5O3
SMILES:	N=c1nc(O)c2ncn(COCCO)c2[nH]1
Mol. weight [g/mol]:	225.20
CAS:	59277-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	-1.571		Crippen Method
mcvol	152.170	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.44	kJ/mol	528.20	NIST Webbook

Sources

Thermal and spectral characterization of a binary mixture (acyclovir and fluocinolone acetonide): Eutectic reaction and inclusion complexes with beta-cyclodextrin:	https://www.doi.org/10.1016/j.tca.2013.03.013
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59277893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume