2-CHLOROADENOSINE

Other names:	Cl AS
	2 ClAdo
	2-Chloroadenosine
	Cl-Ado
	2-chloroadenosinehemihydrate
Inchi:	InChI=1S/C10H12ClN5O4/c11-10-14-7(12)4-8(15-10)16(2-13-4)9-6(19)5(18)3(1-17)20-9
InchiKey:	BIXYYZIIJIXVFW-UHFFFAOYSA-N
Formula:	C10H12ClN5O4
SMILES:	Nc1nc(Cl)nc2c1ncn2C1OC(CO)C(O)C1O
Mol. weight [g/mol]:	301.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Cheméo Relay (1.0)
logp	-1.327		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
tf	488.19	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146770&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point