TCN

Inchi: InChI=1S/C13H16N6O4/c1-18-11-7-5(10(14)17-18)2-19(12(7)16-4-15-11)13-9(22)8(21)6(3-20)23-13/h2,4,6,8-9,13,20-22H,3H2,1H3,(H2,14,17)/t6-,8-,9-,13-/m1/s1

InchiKey: HOGVTUZUJGHKPL-RMXKWMARSA-N

Formula: C13H16N6O4

SMILES: CN1N=C(N)c2cn(C3OC(CO)C(O)C3O)c3ncnc1c23

Mol. weight [g/mol]: 320.30

CAS: 35943-35-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	-1.887		Crippen Method
mcvol	212.450	ml/mol	McGowan Method
rinpol	1891.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35943352&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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