Urea,] 1,1'-trimethylenebis[3-(1,2,3,4-tetrahydro-2,4-diox

Inchi: InChI=1S/C13H16N8O6/c22-8-6(4-16-12(26)20-8)18-10(24)14-2-1-3-15-11(25)19-7-5-17-13(27)21-9(7)23

InchiKey: BFRBOINJWQGXAE-UHFFFAOYSA-N

Formula: C13H16N8O6

SMILES: OC(=NCCCN=C(O)Nc1cnc(O)nc1O)Nc1cnc(O)nc1O

Mol. weight [g/mol]: 380.32

CAS: 96432-16-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.61		Crippen Method
logp	-0.169		Crippen Method
mcvol	252.970	ml/mol	McGowan Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96432165&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume