

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
InchiKey:	BFRBOINJWQGXA-EUHFFFAOYSA-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/ci9903071

Legend

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

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