2-(Hexamethyleneimino)ethanol

Other names:	2-(n-Hexamethyleneimino)ethanol
	N-(«beta»-Hydroxyethyl)hexamethyleneimine
	1H-Azepine-1-ethanol, hexahydro-
	Hexahydro-1H-azepine-1-ethanol
	N-(2-Hydroxyethyl)hexamethyleneimine
	2-(1-azoniacyclohept-1-yl)ethanol
	2-(azepan-1-yl)ethanol
Inchi:	InChI=1S/C8H17NO/c10-8-7-9-5-3-1-2-4-6-9/h10H,1-8H2
InchiKey:	VMRYMOMQCYSPHS-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	OCCN1CCCCCC1
Mol. weight [g/mol]:	143.23
CAS:	20603-00-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.90		Crippen Method
logp	0.855		Crippen Method
mcvol	128.570	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20603003&Units=SI

Legend

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

mcvol: McGowan's characteristic volume