N-beta-hydroxyethyl-n,n'-bis-(4-(6-methyl)-1,3,3a,7

Inchi:	InChI=1S/C16H20N10O/c1-11-7-13(25-15(22-11)18-9-20-25)17-3-4-24(5-6-27)14-8-12(2
InchiKey:	BRPFGTWIGUWOBJ-UHFFFAOYSA-N
Formula:	C16H20N10O
SMILES:	Cc1cc(NCCN(CCO)c2cc(C)nc3ncnn23)n2ncnc2n1
Mol. weight [g/mol]:	368.40
CAS:	111472-54-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	0.090		Crippen Method
mcvol	264.130	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=C111472549&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

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