Ethanol, 2-[(n-methyl-n-purin-2-yl)amino]-

Inchi: InChI=1S/C8H11N5O/c1-13(2-3-14)8-9-4-6-7(12-8)11-5-10-6/h4-5,14H,2-3H2,1H3,(H,9,1
InchiKey: PEPIMBKCCHEOGN-UHFFFAOYSA-N
Formula: C8H11N5O
SMILES: CN(CCO)c1ncc2[nH]cnc2n1
Mol. weight [g/mol]: 193.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	-0.700		Crippen Method
mcvol	140.430	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008231&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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