2-(1-Hydroxy-1-methylethyl)-5-(1-methylethyl)pyra

Inchi: InChI=1S/C10H16N2O/c1-7(2)8-5-12-9(6-11-8)10(3,4)13/h5-7,13H,1-4H3
InchiKey: SEQOBFCOIPROTR-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: CC(C)c1cnc(C(C)(C)O)cn1
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	1.827		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1326.00		NIST Webbook
rinpol	1326.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R412805&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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.