3-Pentanol, 2-(2-benzimidazolyl)-2,4-dimethyl-

Inchi: InChI=1S/C14H20N2O/c1-9(2)12(17)14(3,4)13-15-10-7-5-6-8-11(10)16-13/h5-9,12,17H,1
InchiKey: NLULLYHCXWKUHC-UHFFFAOYSA-N
Formula: C14H20N2O
SMILES: CC(C)C(O)C(C)(C)c1nc2ccccc2[nH]1
Mol. weight [g/mol]: 232.32
CAS: 116465-68-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	2.375		Crippen Method
mcvol	195.030	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=C116465680&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