1-(2-methyl-5-nitroimidazol-1-yl)propan-2-ol

Inchi: InChI=1S/C7H11N3O3/c1-5(11)4-9-6(2)8-3-7(9)10(12)13/h3,5,11H,4H2,1-2H3
InchiKey: KPQZUUQMTUIKBP-UHFFFAOYSA-N
Formula: C7H11N3O3
SMILES: Cc1ncc([N+](=O)[O-])n1CC(C)O
Mol. weight [g/mol]: 185.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Aqueous Solubility Prediction Method
logp	0.481		Crippen Method
mcvol	133.280	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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