5-(2-Hydroxypropyl)-hygrine

Inchi: InChI=1S/C11H21NO2/c1-8(13)6-10-4-5-11(12(10)3)7-9(2)14/h8,10-11,13H,4-7H2,1-3H3
InchiKey: UBTBXKBPQCPOTA-UHFFFAOYSA-N
Formula: C11H21NO2
SMILES: CC(=O)CC1CCC(CC(C)O)N1C
Mol. weight [g/mol]: 199.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	1.199		Crippen Method
mcvol	172.410	ml/mol	McGowan Method
rinpol	1452.00		NIST Webbook
rinpol	1451.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R509865&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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