5-(2-Hydroxypropionyl)-6,7-dimethyl-2,3-dihydro-1

Inchi: InChI=1S/C12H17NO2/c1-7-8(2)11(12(15)9(3)14)13-6-4-5-10(7)13/h9,14H,4-6H2,1-3H3
InchiKey: ZCNNVEPQSPOCJM-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: Cc1c(C)c(C(=O)C(C)O)n2c1CCC2
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	1.615		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R312042&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

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