5-Ethyl-5-methyl-2-(1-methylethyl)-4-isobutanoyl-1

Inchi: InChI=1S/C12H22N2O2/c1-7-12(6)14(11(15)9(4)5)13-10(16-12)8(2)3/h8-9H,7H2,1-6H3
InchiKey: RFHOEJDUAIQBDY-UHFFFAOYSA-N
Formula: C12H22N2O2
SMILES: CCC1(C)OC(C(C)C)=NN1C(=O)C(C)C
Mol. weight [g/mol]: 226.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	2.597		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
rinpol	1340.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116760&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