5,5-Diethyl-2-(1-methylethyl)-4-isobutanoyl-1,3,4-o

Inchi: InChI=1S/C13H24N2O2/c1-7-13(8-2)15(12(16)10(5)6)14-11(17-13)9(3)4/h9-10H,7-8H2,1
InchiKey: HJQQURNRLBEHHW-UHFFFAOYSA-N
Formula: C13H24N2O2
SMILES: CCC1(CC)OC(C(C)C)=NN1C(=O)C(C)C
Mol. weight [g/mol]: 240.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.987		Crippen Method
mcvol	206.270	ml/mol	McGowan Method
rinpol	1410.00		NIST Webbook

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=R116631&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
rinpol: Non-polar retention indices