

2-Pyrazoline, 3-butyl-5,5-dimethyl, N-acetyl

Inchi: InChI=1S/C11H20N2O/c1-5-6-7-10-8-11(3,4)13(12-10)9(2)14/h5-8H2,1-4H3
InchiKey: BWZRQTBISYLORC-UHFFFAOYSA-N
Formula: C11H20N2O
SMILES: CCCCC1=NN(C(C)=O)C(C)(C)C1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	2.563		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
rinpole	1402.00		NIST Webbook
rinpole	1402.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R322940&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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