

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

Inchi: InChI=1S/C9H16N2O/c1-5-9(4)6-7(2)10-11(9)8(3)12/h5-6H2,1-4H3
InchiKey: XJCKUHKNAUNIFP-UHFFFAOYSA-N
Formula: C9H16N2O
SMILES: CCC1(C)CC(C)=NN1C(C)=O
Mol. weight [g/mol]: 168.24

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.10 | | Crippen Method |
| logp | 1.783 | | Crippen Method |
| mcvol | 144.040 | ml/mol | McGowan Method |
| rinpola | 1222.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R322980&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/59-938-6/2-Pyrazoline-5-ethyl-3-5-dimethyl-N-acetyl.pdf>

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