

2-Pyrazoline, 4,4-dimethyl-5-isopropyl, N-acetyl

| | |
|----------------------|---|
| Inchi: | InChI=1S/C10H18N2O/c1-7(2)9-10(4,5)6-11-12(9)8(3)13/h6-7,9H,1-5H3 |
| InchiKey: | YEFOHIBWDZJNMN-UHFFFAOYSA-N |
| Formula: | C10H18N2O |
| SMILES: | CC(=O)N1N=CC(C)(C)C1C(C)C |
| Mol. weight [g/mol]: | 182.26 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.03 | | Crippen Method |
| logp | 1.885 | | Crippen Method |
| mcvol | 158.130 | ml/mol | McGowan Method |
| rinpol | 1270.00 | | NIST Webbook |
| rinpol | 1270.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R322960&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| rinpol: | Non-polar retention indices |

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