

Piperazine, 1,4-diacetyl-

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|-----------------------------|---|
| Other names: | Benzylpiperazine-M (piperazine), 2AC |
| Inchi: | InChI=1S/C8H14N2O2/c1-7(11)9-3-5-10(6-4-9)8(2)12/h3-6H2,1-2H3 |
| InchiKey: | NBQBICYRKOTWRR-UHFFFAOYSA-N |
| Formula: | C8H14N2O2 |
| SMILES: | CC(=O)N1CCN(C(C)=O)CC1 |
| Mol. weight [g/mol]: | 170.21 |
| CAS: | 18940-57-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | 0.24 | | Crippen Method |
| logp | -0.303 | | Crippen Method |
| mcvol | 135.820 | ml/mol | McGowan Method |
| rinpol | 1780.00 | | NIST Webbook |
| rinpol | 1780.00 | | NIST Webbook |
| rinpol | 1750.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C18940573&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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<https://www.cheméo.com/cid/21-903-5/Piperazine-1-4-diacetyl.pdf>

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