

5-methyl-2,3-bis(1'-pyrrolidinyl)-2-cyclopenten-1-one

Other names: 5-Methyl-2,3-bis-(1-pyrrolidinyl)-2-cyclopenten-1-one
Inchi: InChI=1S/C14H22N2O/c1-11-10-12(15-6-2-3-7-15)13(14(11)17)16-8-4-5-9-16/h11H,2-10H
InchiKey: SQSLZARCXRKCIB-UHFFFAOYSA-N
Formula: C14H22N2O
SMILES: CC1CC(N2CCCC2)=C(N2CCCC2)C1=O
Mol. weight [g/mol]: 234.34

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.39 | | Crippen Method |
| logp | 1.998 | | Crippen Method |
| mcvol | 192.770 | ml/mol | McGowan Method |
| ripol | 2975.00 | | NIST Webbook |
| ripol | 2975.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U366035&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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