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

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,2-10
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