1,2-bis-(1-Pyrrolidinyl)-1-buten-3-one

Inchi: InChI=1S/C12H20N2O/c1-10(15)12(14-7-2-3-8-14)9-11-5-4-6-13-11/h9,11,13H,2-8H2,1H

InchiKey: KIELAOHVFOBDLD-XFXZXTDPSA-N

Formula: C12H20N2O

SMILES: CC(=O)C(=CC1CCCN1)N1CCCC1

Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	1.307		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
ripol	2726.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R532459&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

ripol: Polar retention indices