1-(2-phenylethyl)-2-formylpyrrol

Inchi: InChI=1S/C13H13NO/c15-11-13-7-4-9-14(13)10-8-12-5-2-1-3-6-12/h1-7,9,11H,8,10H2
InchiKey: ITWVWJWDKXWQFS-UHFFFAOYSA-N
Formula: C13H13NO
SMILES: O=Cc1cccn1CCc1ccccc1
Mol. weight [g/mol]: 199.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.543		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
ripol	2557.00		NIST Webbook
ripol	2557.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492707&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

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