

1-Ethanone, 2-hydroxy, 1-(4-dimethylaminophenyl)-2-(2-furyl)

Inchi: InChI=1S/C14H15NO3/c1-15(2)11-7-5-10(6-8-11)13(16)14(17)12-4-3-9-18-12/h3-9,14,17
InchiKey: PBVNGLICPDQGAQ-UHFFFAOYSA-N
Formula: C14H15NO3
SMILES: CN(C)c1ccc(C(=O)C(O)c2ccco2)cc1
Mol. weight [g/mol]: 245.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.11		Crippen Method
logp	2.262		Crippen Method
mcvol	188.190	ml/mol	McGowan Method
rinpol	2309.00		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=R121074&Units=SI>

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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