6/28/2018 Chemicalize

Basic properties

Input	COc1cccc(c1)Nc2c3ccccc3ncn2.Cl
Molar mass	287.75 g/mol
Exact mass	287.0825398 Da
Formula	C ₁₅ H ₁₄ CIN ₃ O
Composition	C (62.61%), H (4.9%), Cl (12.32%), N (14.6%), O (5.56%)
Lipinski's rule of five	✓

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pKa

Strongest acidic pKa 15.62

Strongest basic pKa 4

