6/28/2018 Chemicalize

Basic properties

Input	c1cc2c(cc10)c3c(o2)C(=0)NCCC3
Molar mass	217.224 g/mol
Exact mass	217.073893218 Da
Formula	C ₁₂ H ₁₁ NO ₃
Composition	C (66.35%), H (5.1%), N (6.45%), O (22.1%)
Lipinski's rule of five	✓

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pKa



9.44

