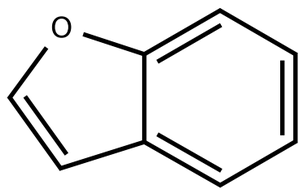
Carbon counting (n=50)

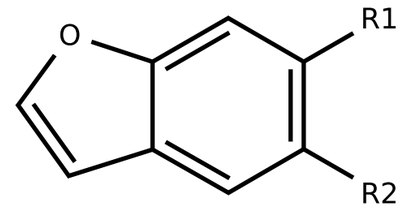
How many carbon atoms are in the molecule [SMILES]



→ 8

SAR Analysis (n=40)

Given [molecular data] determine the score of [SMILES]

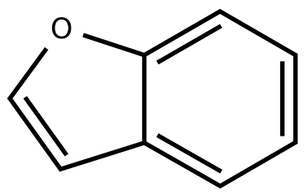


R_1	R_2	Score
Cl	F	87
Br	F	160
Cl	Cl	68
Br	Cl	?

→ 141

Ring counting (n=48)

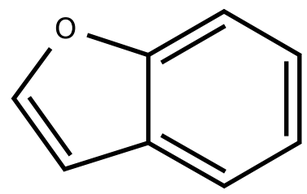
How many rings are in the molecule [SMILES]



→ 2

SMILES to IUPAC (n=200*)

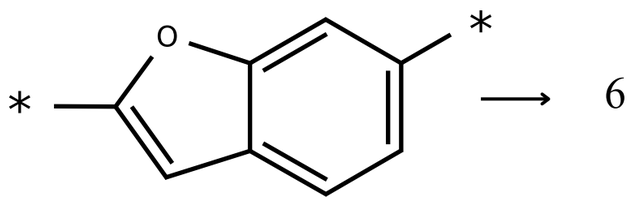
Write the IUPAC name of the molecule [SMILES]



→ 1-benzofuran

Shortest path (n=108*)

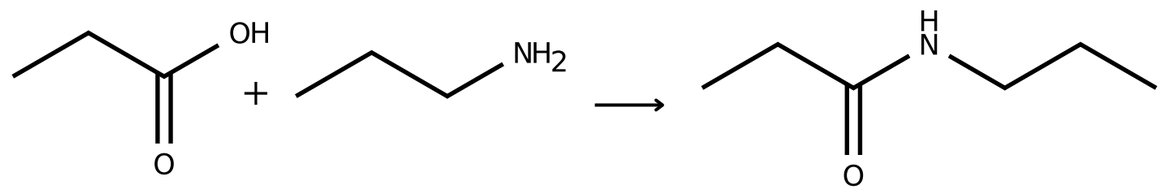
Count bonds between the dummy atoms [SMILES]



→ 6

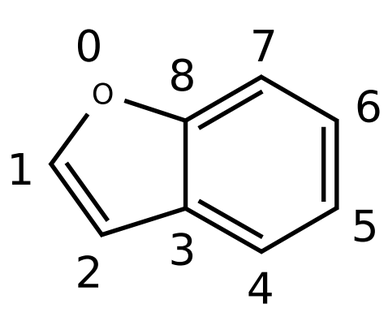
Product of reaction (n=90*)

Write the product of reaction [SMILES 1] + [SMILES 2] as a SMILES string

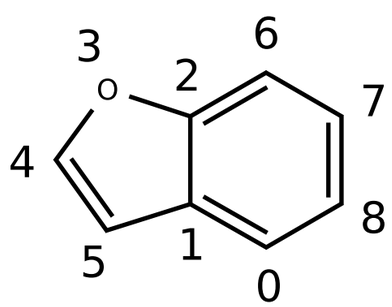


Atom mapping (n=184*)

Map the atoms from [SMILES 1] to [SMILES 2]



o1ccc2ccccc12



c1c2c(occ2)ccc1

→ [(0,3),(1,4),(2,5),(3,1),(4,0),(5,8),(6,7),(7,6),(8,2)]

NMR Elucidation (n=76)

Write the SMILES string of the molecule consistent with this data [Formula] [^{1}H NMR] [^{13}C NMR]

Formula	1H NMR	13C NMR
C7H7NO2	δ 6.89 (2H, ddd, J = 8.5, 1.1, 0.4 Hz), 7.73 (2H, ddd, J = 8.5, 1.7, 0.4 Hz).	δ 114.3 (2C, s), 118.7 (1C, s), 132.8 (2C, s), 151.4 (1C, s), 167.1 (1C, s).

→