



>>Entry Name: 3,5-Dimethyl-1*H*-pyrrole-2-carboxylic acid

Synonym(s): 2,4-Dimethylpyrrole-5-carboxylic acid

CAS Registry Number: 4513-93-3

Structure by analogy with 2,4-Dimethyl-1*H*-pyrrole-3-carboxylic acid, [HHX85-H](#)

Molecular Formula: C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 139.154

Accurate Mass: 139.063329

Percentage Composition: C 60.42%; H 6.52%; N 10.07%; O 23.00%

Melting Point: Mp 137 dec.°

pK<sub>a</sub> Value: pK<sub>a</sub> 5.7

Other Data: Dec. by boiling H<sub>2</sub>O

>>Derivative: Me ester

CAS Registry Number: 74999-36-3

Molecular Formula: C<sub>8</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 153.18

Accurate Mass: 153.078979

Percentage Composition: C 62.73%; H 7.24%; N 9.14%; O 20.89%

Melting Point: Mp 94-96°

>>Derivative: Et ester

CAS Registry Number: 2199-44-2

Molecular Formula: C<sub>9</sub>H<sub>13</sub>NO<sub>2</sub>

Molecular Weight: 167.207

Accurate Mass: 167.094629

Percentage Composition: C 64.65%; H 7.84%; N 8.38%; O 19.14%

Melting Point: Mp 125°

Aldrich: 28892-6

Rare Chemicals Library: S10699-2

>>Derivative: Et ester, picrate

Physical Description: Red cryst. (EtOH)

Melting Point: Mp 99°

>>Derivative: Benzyl ester

CAS Registry Number: 40236-19-9

Molecular Formula: C<sub>14</sub>H<sub>15</sub>NO<sub>2</sub>

Molecular Weight: 229.278

Accurate Mass: 229.110279

Percentage Composition: C 73.34%; H 6.59%; N 6.11%; O 13.96%

Physical Description: Cryst. (CH<sub>2</sub>Cl<sub>2</sub>/hexane)

Melting Point: Mp 102-103°

>>Derivative: Amide

CAS Registry Number: 131475-05-3

Molecular Formula: C<sub>7</sub>H<sub>10</sub>N<sub>2</sub>O

Molecular Weight: 138.169

Accurate Mass: 138.079313

Percentage Composition: C 60.85%; H 7.29%; N 20.27%; O 11.58%

Physical Description: Cryst. (Et<sub>2</sub>O)

Melting Point: Mp 162-163°