



>>Entry Name: 4-Isocyanatobenzoic acid, 9Cl

CAS Registry Number: 46112-47-4

Molecular Formula:  $C_8H_5NO_3$

Molecular Weight: 163.132

Accurate Mass: 163.026944

Percentage Composition: C 58.90%; H 3.09%; N 8.59%; O 29.42%

>>Derivative: Me ester

CAS Registry Number: 23138-53-6

Molecular Formula:  $C_9H_7NO_3$

Molecular Weight: 177.159

Accurate Mass: 177.042594

Percentage Composition: C 61.02%; H 3.98%; N 7.91%; O 27.09%

Melting Point: Mp 48°

Boiling Point: Bp<sub>8</sub> 120°

>>Derivative: Et ester

CAS Registry Number: 30806-83-8

Molecular Formula:  $C_{10}H_9NO_3$

Molecular Weight: 191.186

Accurate Mass: 191.058244

Percentage Composition: C 62.82%; H 4.74%; N 7.33%; O 25.11%

Melting Point: Mp 30-32°

Boiling Point: Bp<sub>17</sub> 144-148°

Aldrich: 15934-4

>>Derivative: Chloride

CAS Registry Number: 3729-21-3

Molecular Formula:  $C_8H_4ClNO_2$

Molecular Weight: 181.578

Accurate Mass: 180.993056

Percentage Composition: C 52.92%; H 2.22%; Cl 19.52%; N 7.71%; O 17.62%

Melting Point: Mp 36-38°

Boiling Point: Bp<sub>1</sub> 95-96°

Aldrich: 37503-9

#### References:

*Aldrich Library of <sup>13</sup>C and <sup>1</sup>H FT NMR Spectra*, 1992, **2**, 1568A; 1568C, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 476B, (*ir*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1432C, (*ir*)

Siefken, W., *Annalen*, 1959, **562**, 75, (*synth, esters*)

Elderfield, R.C. *et al.*, *Croat. Chem. Acta*, 1964, **36**, 33, (*Et ester*)

Iwakura, Y. *et al.*, *J.O.C.*, 1966, **31**, 142, (*synth, ir, chloride*)