Sadtler
Standard
Infrared
Grating Spectra

Volumes 39-40 38001-40000 The publication of the physical data of the Sadtler Standard Spectra and the Sadtler Commercial Spectra is intended to be descriptive. The samples of the materials represented have come generally from other sources than our own laboratories and frequently without the donors' knowledge of their part in this publication.

On the other hand every effort is made by Sadtler Research Laboratories, Inc. to assure the reliability of the published spectra. When improved data is available or errors are called to our attention we revise and reissue the proper replacement spectra.

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Researchers Editors & Malbhers

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SADTLER STANDARD GRATING SPECTRA UPDATE VOLUME -- REISSUED PRISM SPECTRA

This volume contains 1000 absorption spectra recorded on a prism spectrophotometer determined in the 2.0 - 15.0 micron region and presented in a linear wavelength vs. percent transmittance format. These spectra were previously published in the Sadtler Standard Prism Spectra collection and are now re-issued and renumbered in the sequence of the Sadtler Standard Grating Spectra to integrate all available infrared data for the user of this publication. While grating spectra are generally preferred by spectroscopists, it is obviously better to have a prism spectrum if it is the only data available.

The spectra were prepared at Sadtler Research Laboratories unless otherwise noted on the spectrum heading, the name of the donor of each compound is also shown on the heading. Although some of the spectra were published over ten years ago and do not always appear to be of optimum quality, they are included in the publication to insure complete coverage of published compounds.

Standard techniques have been developed in our laboratories to insure that the spectra published are of the best possible quality and reproducible for comparison and identification purposes. The preferred sample preparation methods are the capillary cell for liquids and the KBr wafer for solids, the spectra obtained are qualitative only. The KBr method is used for solids since it is a standard technique and requires a small sample amount for preparation of good spectra, leaving the remainder for further analytical investigation. A paper describing the preparation procedure entitled Improved KBr Techniques by Traude and Philip Sadtler is available from our laboratories.

When the KBr method cannot be used for solids due to reaction with the sample, the Split Mull technique is used; the sample is mulled in mineral oil and the entire spectrum is scanned, then a perfluorinated hydrocarbon mull is prepared and scanned in the 3.0 - 3.8 and 6.6 - 7.4 micron regions. This provides a complete spectrum of the compound.

Liquid samples and low melting solids are generally determined using capillary cells.

Each spectrum is clearly labelled with the sample preparation technique used.

The following five indexes accompany the Sadtler Standard Spectra:

Alphabetical Index Molecular Formula Index Chemical Classes Index Numerical Index Spec-Finder

In each of the first four indexes the grating spectrum numbers of compounds are cross-referenced to their corresponding numbers in the Sadtler Standard collections of Ultraviolet and Nuclear Magnetic Resonance Spectra. A reissued prism spectrum is always signified by a P suffix to the number in the grating column of each index.

The final index, the Spec-Finder, provides a means of identifying spectra of unknown compounds by comparison with the coded peaks of the references.

WE SUGGEST THAT THE INTRODUCTIONS TO THE VARIOUS INDEXES BE READ CAREFULLY TO ASSURE THEIR BEST UTILIZATION.

3-ETHYL-5-[(p-METHOXYPHENOXY)METHYL]-2-OXAZOLIDINONE

38001P

C13H17NO4

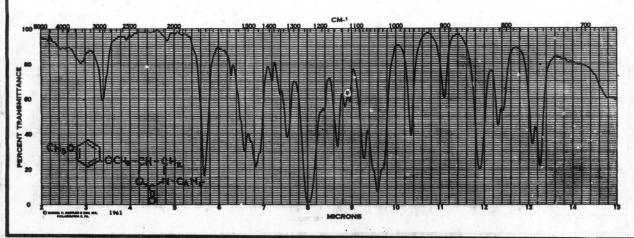
Mol. Wt. 251.28

M.P. 80-81°C

Source of Sample: C. Lunsford, A. H. Robins Co., Inc.

Richmond, Virginia

KBr Wafer



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5-[(3,5-DIMETHOXYPHENOXY)METHYL]-2-OXAZOLIDINONE

38002P

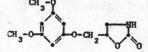
C12H15NO5

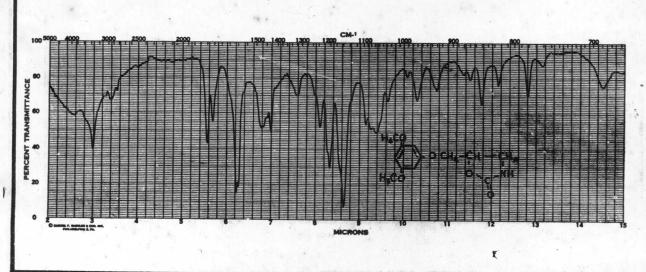
Mol. Wt. 253.26

M.P. 124-125°C

Source of Sample: C. Lunsford, A. H. Robins Co., Inc.

Richmond, Virginia







3-BENZYL-5-[(o-METHOXYPHENOXY)METHYL]-2-OXAZOLIDINONE

C18H19NO4

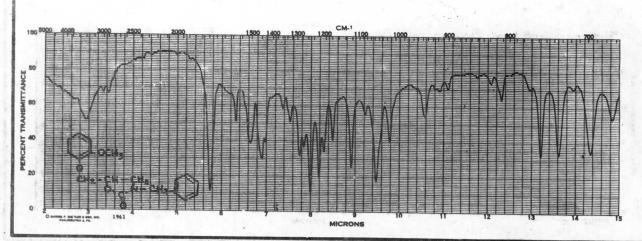
Mol. Wt. 313.36

M.P. 59-59.5°C

Source of Sample: C. Lunsford, A. H. Robins Co., Inc.

Richmond, Virginia

KBr Wafer



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38004P

5-[(p-BROMOPHENOXY)METHYL]-2-OXAZOLIDINONE

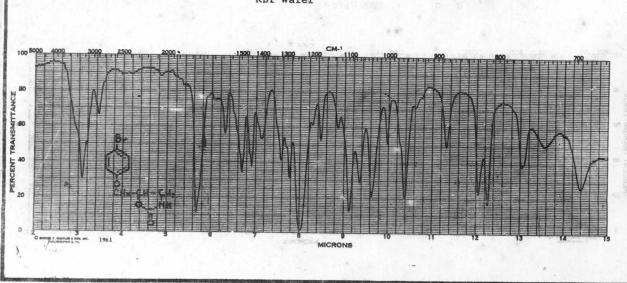
C₁₀H₁₀BrNO₃

Mol. Wt. 272.11

M.P. 153-154°C

Source of Sample: C. Lunsford, A. H. Robins Co., Inc.

Richmond, Virginia



5-[(2,3,5-TRIMETHYLPHENOXY)METHYL]-2-OXAZOLIDINONE

C13H17NQ32

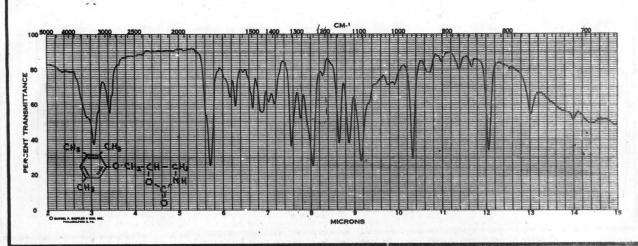
Mol. Wt. 235.29

M.P. 125-126°C

78,20

Source of Sample: C. Lunsford, A. H. Robins Co., Inc. Richmond, Virginia

KBr Wafer



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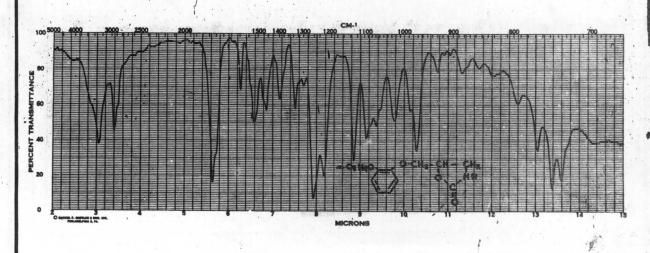
5-[(o-BUTOXYPHENOXY)METHYL]-2-OXAZOLIDINONE

38006P

Mol. Wt. 265.31

M.P. 62-63°C

Source of Sample: C. Lunsford, A. H. Robins Co., Inc. Richmond, Virginia



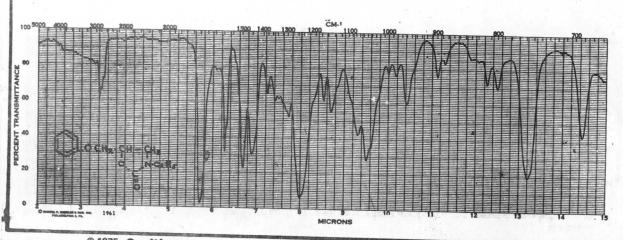
 $C_{12}H_{15}NO_3$

Mol. Wt. 221.26

M.P. 43-44°C

Source of Sample: C. Lunsford, A. H. Robins Co., Inc. Richmond, Virginia

KBr Wafer



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38008P

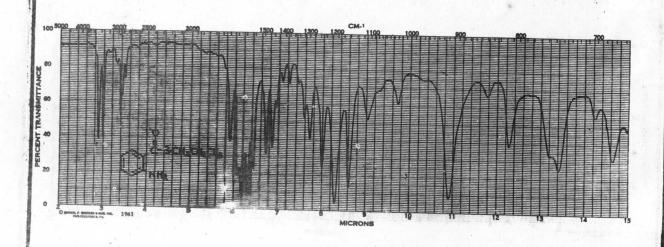
THIOANTHRANILIC ACID, S-PROPYL ESTER

C₁₀H₁₃NOS

Mol. Wt. 195.29

Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

Capillary Cell: Neat

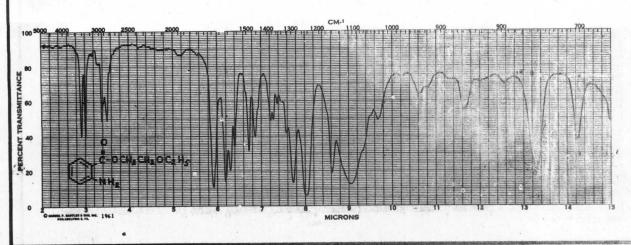


C11H15NO3

Mol. Wt. 209.25

Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

Capillary Cell: Neat



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THIOANTHRANILIC ACID, S-BENZYL ESTER

38010P

C14H13NOS

Mol. Wt. 243.33

Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

Capillary Cell: Neat





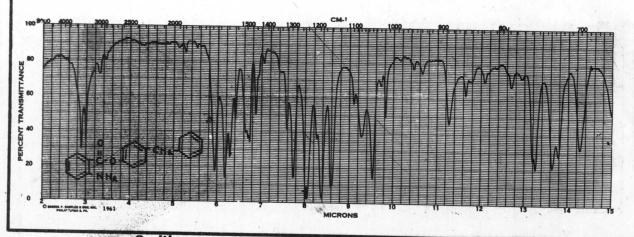
ANTHRANILIC ACID, p-BENZYLPHENYL ESTER

 $^{\rm C}20^{\rm H}17^{\rm NO}2$

Mol. Wt. 303.36

Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

KBr Wafer



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38012P

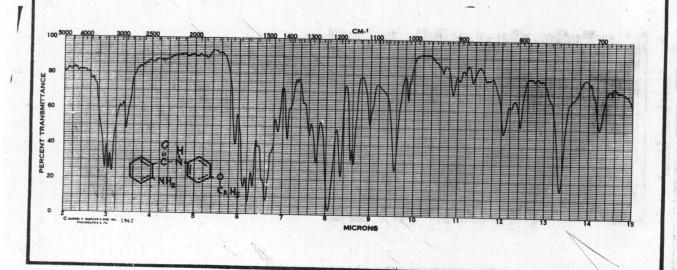
2-AMINO-p-BENZOPHENETIDIDE

C₁₅H₁₆N₂O₂

Mol. Wt. 256.31

Source of Sample

R. Staiger, Ursinus College Collegeville, Pennsylvania

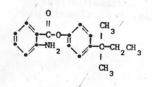


ANTHRANILIC ACID, p-tert-PENTYLPHENYL ESTER

38013P

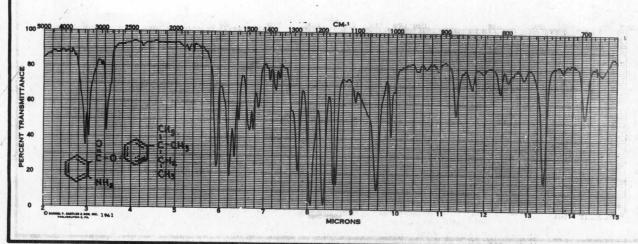
C18H21NO2

Mol. Wt. 283.37



Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

KBr Wafer



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ANTHRANILIC ACID, 2,2,2-TRIFLUOROETHYL ESTER

38014P

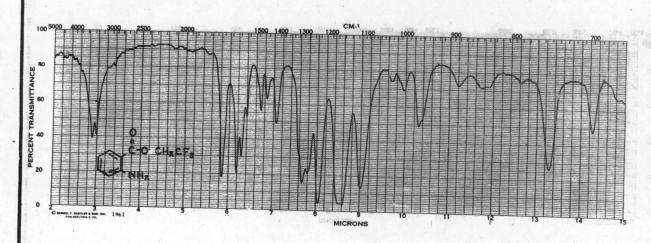
C9H8F3NO2

Mol. Wt. 219.16



Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

KBr Wafer





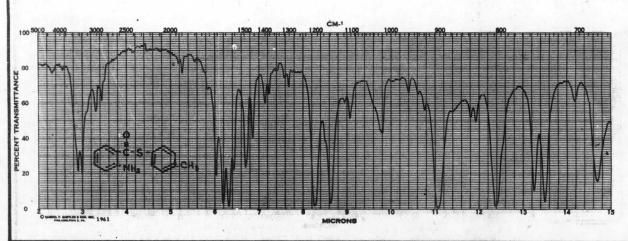
THIOANTHRANILIC ACID, S-p-TOLYL ESTER

C₁₄H₁₃NOS

Mol. Wt. 243.33

Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania

KBr Wafer



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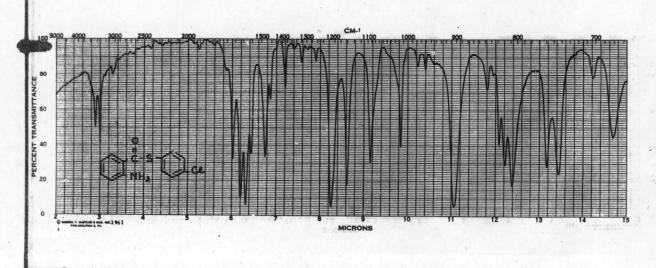
38016P

THIOANTHRANILIC ACID, S-(p-CHLOROPHENYL) ESTER

C₁₃H₁₀ClNOS

Mol. Wt. 263.75

Source of Sample: R. Staiger, Ursinus College Collegeville, Pennsylvania



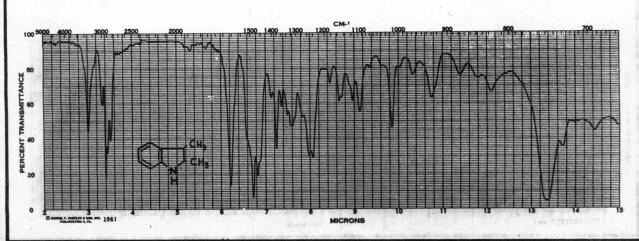
cis-2,3-DIMETHYLINDOLINE

C₁₀H₁₃N

Mol. Wt. 147.22

Source of Sample: Aldrich Chemical Company, Inc. Milwaukee, Wisconsin

Capillary Cell: Neat



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6-METHYL-2-PYRIDYL PHENYL KETONE

38018P

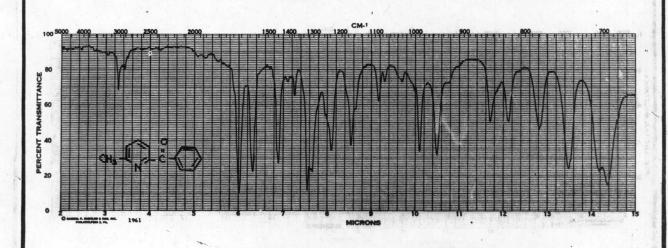
C13H11NO

Mol. Wt. 197.24

Source of Sample: Aldrich Chemical Company, Inc.

Milwaukee, Wisconsin

Capillary Cell: Neat



1.570 19

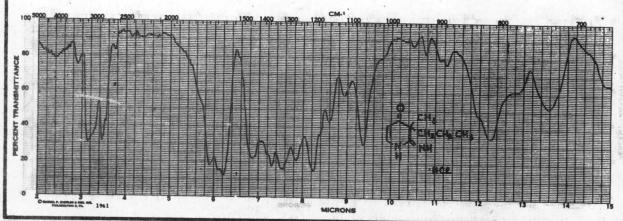
C9H14N2O.HC1

Mol. Wt. 202.69

Source of Sample: F. Hoffmann-La Roche & Co., Ltd.

Basle, Switzerland

Capillary Cell: Neat



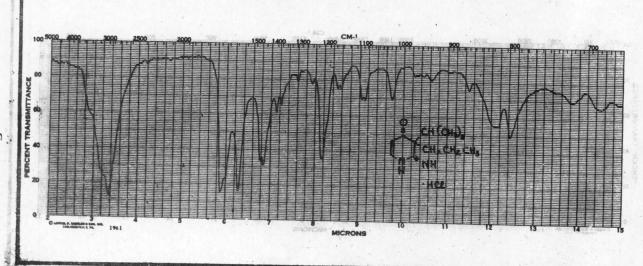
© 1975 Sadtler Research Laboratories, Inc., Subsidiary of Block Engineering, Inc.

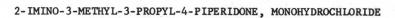
38020P

2,3-DIHYDRO-2-IMINO-3-ISOPROPYL-3-PROPYL-4(1H)-PYRIDONE, MONOHYDROCHLORIDE

C₁₁H₁₈N₂O·HC1 Mol. Wt. 230.74

Source of Sample: F. Hoffmann-La Roche & Co., Ltd. Basle, Switzerland





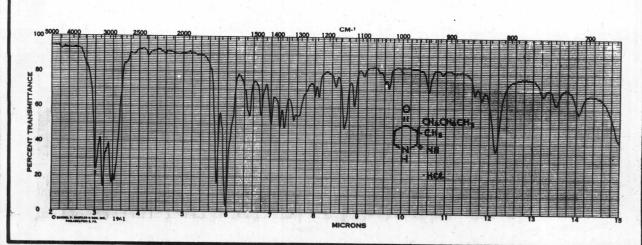
 $C_9H_{16}N_2O\cdot HC1$

Mol. Wt. 204.70

Source of Sample: F. Hoffmann-La Roche & Co., Ltd.

Basle, Switzerland

KBr Wafer



Sadtler Research Laboratories, Inc., Subsidiary of Block Engineering, Inc.

3,3-DIETHYL-2,4-PIPERIDINEDIONE

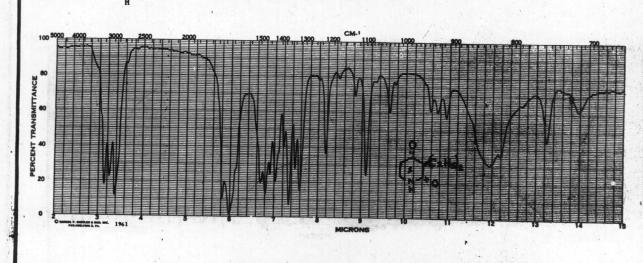
38022P

C9H15NO2

Mol. Wt. 169.23



Source of Sample: F. Hoffmann-La Roche & Co., Ltd. Basle, Switzerland



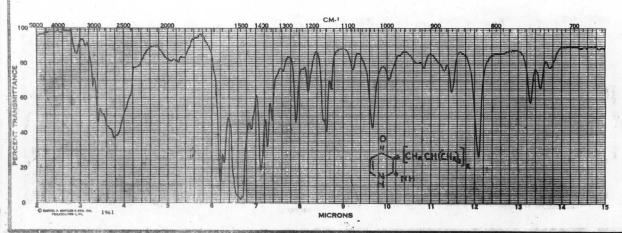
2,3-DIHYDRO-3,3-DIISOBUTYL-2-IMINO-4(1H)-PYRIDONE

 $C_{13}H_{22}N_2O$

Mol. Wt. 222.33

Source of Sample: F. Hoffmann-La Roche & Co., Ltd. Basle, Switzerland

KBr Wafer



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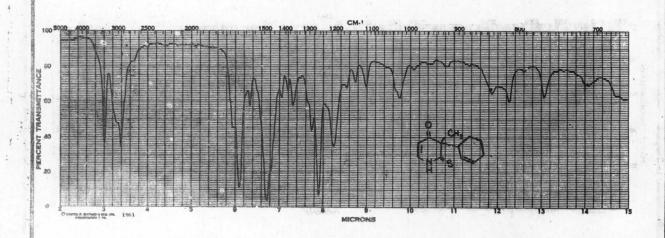
38024P

3-(2-CYCLOHEXENYL)-3-METHYL-2-THIOXO-4(1H)-PYRIDONE

C₁₂H₁₅NOS

Mol. Wt. 221.32

Source of Sample: F. Hoffmann-La Roche & Co., Ltd. Basle, Switzerland





3-ALLYL-2-AMINO-3-PROPYL-4(3H)-PYRIDONE

 $^{\mathrm{C}}_{11}^{\mathrm{H}}_{16}^{\mathrm{N}}_{2}^{\mathrm{O}}$

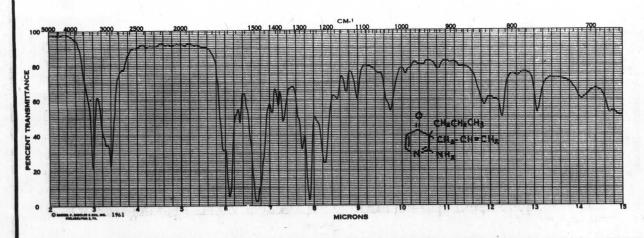
Mol. Wt. 192.26

CH, CH, CH,

Source of Sample: F. Hoffmann-La Roche & Co., Ltd.

Basle, Switzerland

KBr Wafer



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3,3-DIETHYL-2,3-DIHYDRO-2-IMINO-4(1H)-PYRIDONE

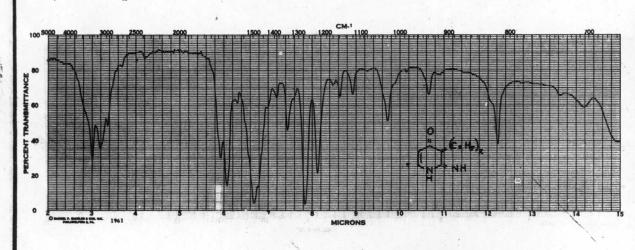
38026P

C9H14N2O Mol. Wt. 166.22



Source of Sample: F. Hoffmann-La Roche & Co., Ltd.

Basle, Switzerland

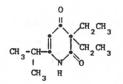




3,3-DIETHYL-6-ISOPROPYL-2,4(1H,3H)-PYRIDINEDIONE

C12H19NO2

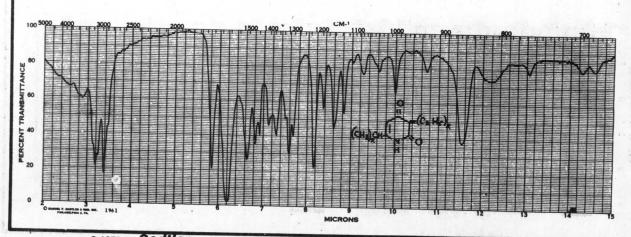
Mol. Wt. 209.29



Source of Sample: F. Hoffmann-La Roche & Co., Ltd.

Basle, Switzerland

KBr Wafer



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38028P

6-THIOURIC ACID

C5H4N4O2S

Mol. Wt. 184.18



Source of Sample: F. Bergmann, Hebrew University Jerusalem, Israel

