Supplementary Material

Synthesis of 4,5,6-trichloropyrimidine-2-carbonitrile from 4,6-dichloro-2-(methylthio)pyrimidine

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Issue in honor of Dr. Jan Bergman

$^1$H NMR of 4,6-bis(benzyloxy)-2-(methylthio)pyrimidine (14)

Current Data Parameters
NAME Kalogirou
EXPNO 287
PROCNO 1

F2 - Acquisition Parameters
Date 2017/02/15
Time 18:33
INSTRUM spect
PROBHD 5 mm PABBO.BB.
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.122588 Hz
AQ 3.2757999 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 294.7 K
D1 1.0000000 sec
TD0 1

== CHANNEL f1 ==
SFO1 500.0361138 MHz
NUC1 1H
F1 12.00 usec
PLW1 14.5000000 W

F2 - Processing parameters
SI 65536
SF 500.0330403 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
$^1$H NMR of 4,6-bis(benzoxyl)-2-(methylsulfonyl)pyrimidine (15)
\[ ^1H \text{NMR of 4,6-bis(benzyloxy)pyrimidine-2-carbonitrile (16)} \]

Current Data Parameters
NAME: Kalogirou
EXPNO: 275
PROCNO: 1

F2 - Acquisition Parameters
Data: 20170359
Time: 3.29
INSTRUM: spect
PROBHD: 5 mm PABBO BB-PULPEOF zg50
TD: 65536
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.132588 Hz
AQ: 3.2767999 sec
RG: 90.3
DW: 50.000 usec
DE: 6.50 usec
TE: 29.72 K
DI: 1.00000000 sec
TD0: 1

CHANNEL f1
SFO1: 500.0361139 MHz
NUC1: 1H
P1: 12.00 usec
PLW1: 14.5000000 W

F2 - Processing parameters
SI: 65536
SF: 500.0330403 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
$^{13}$C NMR of 4,6-bis(benzyloxy)pyrimidine-2-carbonitrile (16)
\textbf{\textsuperscript{1}H NMR of 4,6-bis(benzyloxy)-5-chloropyrimidine-2-carbonitrile (17)}

![NMR spectrum]

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\textbf{Current Data Parameters}

- **NAME**: Kalamnou
- **EXPNO**: 275
- **PROCNO**: 1

\textbf{F2 - Acquisition Parameters}

- **Date**: 20170113
- **Time**: 20:18
- **INSTRUM**: spect
- **PROBHD**: 5 mm PABBO BB
- **TD**: 65536
- **SOLVENT**: CDCl3
- **DS**: 2
- **SWH**: 10000.000 Hz
- **FIDRES**: 0.152988 Hz
- **AQ**: 3.27670999 sec
- **RG**: 114
- **DW**: 50.000 usec
- **DE**: 6.50 usec
- **TE**: 295.2 K
- **D1**: 1.00000000 sec
- **TD0**: 1

\textbf{CHANNEL f1}

- **SFO1**: 500.366158 MHz
- **NUC1**: \textit{IH}
- **P1**: 12.00 usec
- **PLW1**: 14.50000000 W

\textbf{F2 - Processing parameters}

- **SI**: 65536
- **SF**: 500.0330403 MHz
- **WDW**: EM
- **SSB**: 0
- **LB**: 0.30 Hz
- **GB**: 0
- **PC**: 1.00

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\[ ^{13}C \text{ NMR of 4,6-bis(benzyloxy)-5-chloropyrimidine-2-carbonitrile (17)} \]

129.0 128.5 128.0

13C NMR of 4,6-bis(benzyloxy)-5-chloropyrimidine-2-carbonitrile (17)

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Current Data Parameters
NAME Kaloigrou
EXPNO 276
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170314
Time 9.19
INSTRUM spect
PROBD HD 5 mm PABBO BB-
PULFROG jmod
TD 55.5
SOLVENT CDC13
NS 1484
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 29.1 K
CNST2 145.000000
CNST1 1.000000
D1 2.00000000 sec
D20 0.00689625 sec
T20 1
--- CHANNEL f1 ---
SFO1 125.7459782 MHz
NUC1 13C
P1 9.00 usec
P2 18.00 usec
PLW1 133.0000000 W
--- CHANNEL f2 ---
SFO2 590.0359300 MHz
NUC2 1H
CPDPRQ wakt16
PCPD2 80.00 usec
PLW2 14.5000000 W
PLW12 0.33624999 W
F2 - Processing parameters
SI 32.68
SF 125.7334968 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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