

## Chemistry Report for Case # P-15-0633

### General

**Submitter:**Firmenich Inc.

**Contact:** Kerry Blissett

**Contact Telephone No.:** (608) 580-6665

**TS No.:** TS15D4

**Chemist:** Roberts, Justin

**Contractor Support:** Y

**PV Init (kg/yr):** ██████████

**PV Max (kg/yr):** ██████████

**Binding Option:**

**Exposure-Based Review:**

**Manufacture:**

**Import:**

**CAS Number:**870515-09-6

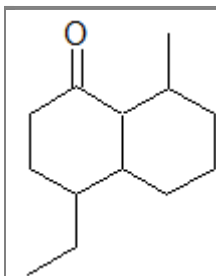
**Chemical Name:**1(2H)-Naphthalenone,  
4-ethyloctahydro-8-methyl-

**Trade Name:**Vetyvalone

**IES Order:**None

**Generic Name:**not  
CBI

### Chemical Structure



### Physical Chemical Properties

**Molecular Formula:**C13 H22

**Molecular Weight:**194.32

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<b>% &lt; 500:</b>	<b>% &lt; 1000:</b>
<b>MP:</b>	<b>MP Estimate:</b> <-20
<b>BP:</b>	<b>BP Pressure:</b> 737.00
<b>BP Estimate:</b> 273	
<b>VP (Torr):</b> 0.012750	<b>VP Estimate (Torr):</b>
<b>Water Solubility (g/L):</b> 0.112000	<b>Water Soluble Estimate (g/L):</b>
<b>Log P:</b> 3.63	<b>Log P Estimate:</b> 4.29
<b>Physical State — Neat:</b> Liquid	<b>Physical State — Manuf:</b> NK - Imported

**Physical State — Processing:** Solution, [REDACTED]  
[REDACTED]

**Physical State — End Use:** Solution, [REDACTED]  
[REDACTED]

### Additional Chemical Info

The PMN material is a mixture of stereoisomers; the submitter provided the following composition for the stereocenters: [REDACTED]  
[REDACTED]

Submitted data: liquid; MP < -20 °C (OECD 102); BP = 272 °C at 737 torr (OECD 103) (NOMO5: 273 °C at 760 torr); VP = 0.01275 torr at 25 °C (OECD 104); WS = 0.0247 g/L (column elution method), 0.112 g/L (OECD 105); log P = 3.63-4.29, the main peaks (90.7%) have log P = 4.23-4.29 (OECD 123), 4.51-4.85 (OECD 117); flash point = 124 °C; autoignition temp. = 255 °C; density = 0.967 g/cc (OECD 109); loc Koc = 3.03-3.06; [REDACTED] The PMN material may undergo base-catalyzed isomerization.

### Uses

**Consumer Use?** Yes  
**Use:** [REDACTED]

**Other Uses:**

[REDACTED]

No other uses found for the PMN material.

**Reaction Description**

The PMN material is imported and no manufacturing information was provided by the submitter. The PMN material may be [REDACTED]

**Pollution Prevention Analysis(P2 Analysis:)**

P2

Claims: 1) Reduction of waste generation: Mixtures containing this chemical, which do not pass specifications, are blended together with other like off-specification materials, and these blends of waste are sold for one-time use as fragrance oils for specific low-value applications. Thus, waste recapture eliminates material from the manufacturing plant. 2) Waste removal & Operation efficiency: When the containers are empty, the covers are re-fastened, without washing, and the containers are removed by a private contractor for incineration of any residue in the container. The vessel in which the new chemical has been mixed/blended is cleaned with hot water and soap solution after processing, and the waste treated on site. Transfer of the mixture containing the new chemical to drums for shipping is accomplished by pumping in a closed system.

**Analogs**

Analogs:

[REDACTED]

**Comments/Telephone Log**

Artifact	Update/Upload Time
[REDACTED]	[REDACTED]