

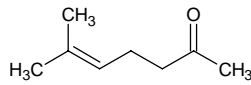
6-methyl-5-hepten-2-one

6-メチル-5-ヘプテン-2-オン

Formula C₈H₁₄O

Mol. Wt. 126.20

CAS No. 110-93-0



SEQ No. 1841 ケトン類

FEMA No. 2707

JECFA No. 1120

| | JFFMA | JECFA | FCC |
|---------------------------|---|-----------------------------------|--------------------------------------|
| Chemical name | 6-methyl-5-hepten-2-one | 6-Methyl-5-hepten-2-one | 6-Methyl-5-hepten-2-one |
| Content (NLT) | 95.0 % (GC) | 97 % | 98.0 % GC(M-1b) |
| Refractive index | 1.435-1.445 (n _{20D}) | 1.435-1.445 (n _{20D}) | 1.438-1.442 (n _{20D}) |
| Specific gravity | 0.847-0.857 (d _{20/20}) | 0.846-0.854 (d _{25/25}) | 0.846-0.851 (d _{25/25}) |
| Acid value (NMT) | | 3.0 | |
| Melting/Congeaing point | | | |
| Angular/Specific rotation | | | |
| Heavy metals (NMT) | | | |
| Solubility in ethanol | | Miscible at room temperature | 1 mL in 2mL 70% alc gives clear soln |
| Other requirements | | | |
| Identification* | IR : 2,3,5,6 MS : 3,4,5 NMR : 1,3,6 | NMR | IR |

*References

- 1: Joint FAO/WHO Expert Committee on Food Additive (JECFA)
- 2: Food Chemicals Codex (FCC)
- 3: 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)
- 4: Wiley's Registry of Mass spectral Database
- 5: NIST/EPA/NIH Mass Spectral Library
- 6: Sigma-Aldrich