

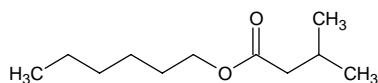
hexyl isovalerate

ヘキシル イソバレレート

Formula C₁₁H₂₂O₂

Mol. Wt. 186.29

CAS No. 10032-13-0



SEQ No. 1208 エステル類

FEMA No. 3500

JECFA No. 199

	JFFMA	JECFA	FCC
Chemical name	hexyl isovalerate	Hexyl 3-methylbutanoate	Hexyl Isovalerate
Content (NLT)	95.0 % (GC)	95.0 %	95.0 % sum of two isomers; isovalerate isomer 92.0% min /GC(M-1b)
Refractive index	1.413-1.423 (n _{20D})	1.417-1.421 (n _{20D})	1.417-1.421 (n _{20D})
Specific gravity	0.854-0.864 (d _{20/20})	0.853-0.857 (d _{25/25})	0.853-0.857 (d _{25/25})
Acid value (NMT)	1.0	2.0	2.0
Melting/Congeeing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol			1 mL in 1 mL 95% alc
Other requirements			
Identification*	IR :1,3,6 MS :4,5 NMR :3	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