

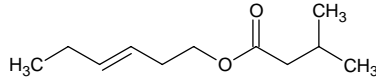
3-hexenyl isovalerate

3-ヘキセニル イソバレレート

Formula C₁₁H₂₀O₂

Mol. Wt. 184.28

CAS No. 10032-11-8



SEQ No. 1169 エステル類

FEMA No. 3498

JECFA No. 202

	JFFMA	JECFA	FCC
Chemical name	3-hexenyl isovalerate	3-Hexenyl 3-methylbutanoate	(Z)-3-Hexenyl Isovalerate
Content (NLT)	95.0 % (GC) sum of isomers	95.0 %	95.0 % sum of two isomers; (Z)- isomer 92.0% min /GC(M1-a)
Refractive index	1.427-1.437 (n _{20D})	1.429-1.435 (n _{20D})	1.429-1.435 (n _{20D})
Specific gravity	0.873-0.883 (d _{20/20})	0.874-0.876 (d _{25/25})	0.872-0.877 (d _{25/25})
Acid value (NMT)	2.0	2.0	2.0
Melting/Congeealing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol			1 mL in 1 mL 95% ethanol
Other requirements			
Identification*	IR :1 MS :4 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