

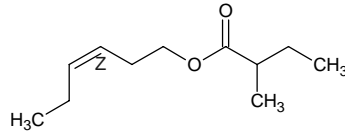
cis-3-hexenyl 2-methylbutyrate

cis-3-ヘキセニル 2-メチルブチレート

Formula C₁₁H₂₀O₂

Mol. Wt. 184.28

CAS No. 53398-85-9



SEQ No. 1133 エステル類

FEMA No. 3497

JECFA No. 211

	JFFMA	JECFA	FCC
Chemical name	cis-3-hexenyl 2-methylbutyrate	3-Hexenyl 2-methylbutanoate	(Z)-3-Hexenyl 2-Methylbutyrate
Content (NLT)	95.0 % (GC)	98 %	95.0 % sum of two isomers; (Z)- isomer 92.0% min /GC(M1-a)
Refractive index	1.429-1.439 (n _{20D})	1.428-1.434 (n _{20D})	1.430-1.434 (n _{20D})
Specific gravity	0.876-0.886 (d _{20/20})	0.876-0.880 (d _{25/25})	0.876-0.880 (d _{25/25})
Acid value (NMT)	1.0		2.0
Melting/Congeeing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol			1 mL in 1 mL 95% ethanol
Other requirements			
Identification*	IR : 1 MS : 4,5 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