

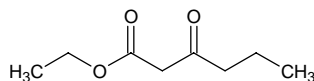
ethyl 3-oxohexanoate

エチル 3-オキソヘキサノエート

Formula C₈H₁₄O₃

Mol. Wt. 158.20

CAS No. 3249-68-1



SEQ No. 788 エステル類

FEMA No. 3683

JECFA No. 602

	JFFMA	JECFA	FCC
Chemical name	ethyl 3-oxohexanoate	Ethyl 3-oxohexanoate	
Content (NLT)	98.0 % (Chem)	96 % with 2-3% ethyl 2-acetyl-3-oxohexanoate	
Refractive index	1.424-1.436 (n _{20D})	1.424-1.436 (n _{20D})	
Specific gravity	0.983-1.000 (d _{20/20})	0.983-1.000 (20°C)	
Acid value (NMT)	1.0		
Melting/Congeealing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol			
Other requirements			
Identification*	IR : 1,3,6 MS : 1,3,4,5 NMR : 1,3,6	NMR, MS, 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