

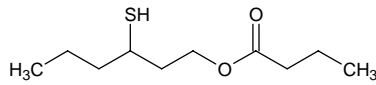
3-mercaptohexyl butyrate

3-メルカプトヘキシル ブチレート

Formula C₁₀H₂₀O₂S

Mol. Wt. 204.33

CAS No. 136954-21-7



SEQ No. 2587 エステル類

FEMA No. 3852

JECFA No. 555

	JFFMA	JECFA	FCC
Chemical name	3-mercaptohexyl butyrate	3-Mercaptohexyl butyrate	
Content (NLT)	98.0 % (GC)	90 %	
Refractive index	1.456-1.462 (n _{20D})	1.459-1.469 (n _{20D})	
Specific gravity	0.963-0.969 (d _{20/20})	0.960-0.965 (d _{25/25})	
Acid value (NMT)	1.0		
Melting/Congeealing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol			
Other requirements			
Identification*	IR :1 MS :1,4,5 NMR :1	IR, MS, NMR	

*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