

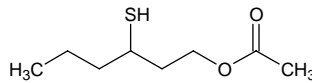
## 3-mercaptohexyl acetate

### 3-メルカプトヘキシル アセテート

Formula C<sub>8</sub>H<sub>16</sub>O<sub>2</sub>S

Mol. Wt. 176.28

CAS No. 136954-20-6



SEQ No. 1543 エステル類

FEMA No. 3851

JECFA No. 554

	JFFMA	JECFA	FCC
Chemical name	3-mercaptohexyl acetate	3-Mercaptohexyl acetate	
Content (NLT)	98.0 % (GC)	81.7 %	
Refractive index	1.455-1.465 (n <sub>20D</sub> )	1.462-1.472 (n <sub>20D</sub> )	
Specific gravity	0.985-0.996 (d <sub>20/20</sub> )	0.991-0.996 (d <sub>25/25</sub> )	
Acid value (NMT)	1.0		
Melting/Congeealing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol			
Other requirements		Also contains min. 8.2% 3-Mercaptohexanol and 9.7% 3-Acetylmercaptohexyl acetate	
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