

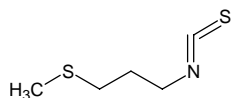
3-(methylthio)propyl isothiocyanate

3-(メチルチオ)プロピル イソチオシアネート

Formula C₅H₉NS₂

Mol. Wt. 147.26

CAS No. 505-79-3



SEQ No. 1891 イソチオシアネート類

FEMA No. 3312

JECFA No. 1564

	JFFMA	JECFA	FCC
Chemical name	3-(methylthio)propyl isothiocyanate	3-Methylthiopropyl isothiocyanate	
Content (NLT)	90.0 % (GC)	98 %	
Refractive index	1.556-1.566 (n _{20D})	1.560-1.566 (n _{20D})	
Specific gravity	1.106-1.116 (d _{20/20})	1.099-1.105 (d _{25/25})	
Acid value (NMT)		1	
Melting/Congeealing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol		Soluble	
Other requirements			
Identification*	IR :3,5,6 MS :3,4,5,6 NMR :1,3,6	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