

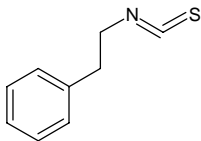
phenethyl isothiocyanate

フェネチル イソチオシアネート

Formula C9H9NS

Mol. Wt. 163.24

CAS No. 2257-09-2



SEQ No. 2114 イソチオシアネート類

FEMA No. 4014

JECFA No. 1563

	JFFMA	JECFA	FCC
Chemical name	phenethyl isothiocyanate	Phenethyl isothiocyanate	
Content (NLT)	97.0 % (GC)	99 %	
Refractive index	1.585–1.595 (n20D)	1.586–1.590 (n20D)	
Specific gravity	1.090–1.100 (d20/20)	1.087–1.097 (d25/25)	
Acid value (NMT)		1	
Melting/Congeaing point			
Angular/Specific rotation			
Heavy metals (NMT)			
Solubility in ethanol		Soluble	
Other requirements			
Identification*	IR : 1,3,6 MS : 1,3,4,5 NMR : 1,3	HNMR IR MS	

*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