

SPECIFICATION

Theobromine

Parameters	Specification
CAS Number	83-67-0
Appearance	White crystalline powder
Molecular Formula	C ₇ H ₈ N ₄ O ₂
Molecular Weight	180.17 g/mol
Boiling Point	400 °C
Melting Point	322 °C
Flash Point	210 °C
Purity	99–99.5%
Refractive Index	1.60
Solubility	Very slightly soluble in water; 0.06 g/100 mL at 25 °C
Uses	Stimulant used in pharmaceutical research and as a natural alkaloid in cacao products; also used as a chemical intermediate

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