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## Typical Product Specifications & Properties

# Guaiazulene

CAS Number: : 489-84-9

Specifications	Limits
Molecular weight	198.30
EINECS	207-701-2
SMILES	<chem>c12c(c(ccc(c1)C(C)C)C)ccc2C</chem>
InChI	1S/C15H18/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h5-10H,1-4H3
InChIKey	FWKQNCXZGNBPFD-UHFFFAOYSA-N
Atmospheric OH Rate Constant	3.43E-10 cm <sup>3</sup> /molecule-sec
Melting Point	31.5 &deg; C
log P (octanol-water)	5.930
Density	0.976 g/mL at 25 &deg;C
Flash Point	>230 &deg;F
Storage Temperature	2-8&deg;C
BRN Number	1365001



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Specifications	Limits
Melting Point	27-29 °C
Boiling Point	153 °C/7 mm Hg
Water solubility	Soluble in alcohol, water, 0.1115 mg/L @ 25°C (est).
Merck	14,4554



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