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## Typical Product Specifications & Properties

# β-Bisabolol

CAS Number: : 15352-77-9

Specifications	Limits
Molecular weight	222.37
InChI	1S/C15H26O/c1-12(2)6-5-7-14(4)15(16)10-8-13(3)9-11-15/h6,8,14,16H,5,7,9-11H2,1-4H3/t14-,15+/m0/s1
InChIKey	WTVHAMTYZJGJLJ-LSDHHAIUSA-N
Molecular weight	156.27
EINECS	216-074-4
SMILES	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O
InChI	1S/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H,4-6H2,1-3H3/t8-,9+,10-/m1/s1
InChIKey	NOOLISFMXDJSKH-KXUCPTDWSA-N
Water solubility	456 mg/L
Henry's Law Constant	1.52E-05 atm-m <sup>3</sup> /mole
Melting Point	35 &deg; C
Boiling Point	212 &deg; C



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Specifications	Limits
log P (octanol-water)	3.4
Atmospheric OH Rate Constant	2.41E-11 cm <sup>3</sup> /molecule-sec
Flash Point	200 &deg;F
Melting Point	34-36 &deg;C
FEMA	2665
Boiling Point	216 &deg;C
Density	0.89 g/mL at 25 &deg;C
Vapor Pressure	0.8 mm Hg ( 20 &deg;C)
Chemical Structure	 59877_59877_β-bisabolol.png chemical structure



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