

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-m3/mole
Melting Point	35 ° C
Boiling Point	212 ° C



Specifications	Limits
log P (octanol-water)	3.4
Atmospheric OH Rate Constant	2.41E-11 cm ³ /molecule-sec
Flash Point	200 °F
Melting Point	34-36 °C
FEMA	2665
Boiling Point	216 °C
Density	0.89 g/mL at 25 °C
Vapor Pressure	0.8 mm Hg (20 °C)