

Typical Product Specifications & Properties

Santonin

CAS Number: : 481-06-1

Specifications	Limits
Molecular weight	246.30
EINECS	207-560-7
SMILES	<chem>C[C@H]1[C@@H]2CC[C@@]3(C)C=CC(=O)C(=C3[C@H]2OC1</chem>
InChI	1S/C15H18O3/c1-8-10-4-6-15(3)7-5-11(16)9(2)12(15)13(10)18-14(8)17/h5,7-8,10,13H,4,6H2,1-3H3/t8-,10-,13-,15-/m0/s1
InChIKey	XJHDMGJURBVLE-BOCCBSBMSA-N
Water solubility	200 mg/L
Melting Point	175 ° C
Henry's Law Constant	5.27E-08 atm-m ³ /mole
Atmospheric OH Rate Constant	5.83E-11 cm ³ /molecule-sec
Vapor Pressure	2.38E-06 mm Hg
log P (octanol-water)	1.780
Refractive Index	-172.5 ° (C=2, CHCl ₃)

Specifications	Limits
Storage Temperature	2-8°C
Melting Point	172-173 °C
Merck	8361