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Typical Product Specifications & Properties

Codeine Alkaloid

CAS Number: : 76-57-3

Specifications	Limits
Molecular weight	299.36
EINECS	200-969-1
SMILES	<chem>COC1ccc2C[C@@H]3[C@@H]4C=C[C@H](O)[C@@H]5Oc1c2[C@]45CCN3C</chem>
InChI	1S/C18H21NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18)9-12(11)19/h3-6,11-13,17,20H,7-9H2,1-2H3
InChIKey	OROGSEYTTFOCAN-UHFFFAOYSA-N
Melting Point	157.5 ° C
Water solubility	9000 mg/L
Henry's Law Constant	7.58E-14 atm-m ³ /mole
pKa Dissociation Constant	8.21
Vapor Pressure	4.15E-09 mm Hg
log P (octanol-water)	1.19
Atmospheric OH Rate Constant	2.43E-10 cm ³ /molecule-sec



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