

Typical Product Specifications & Properties

Cafestol

CAS Number: : 469-83-0

Specifications	Limits
Molecular weight	316.43
SMILES	<chem>C1[C@@H]2C[C@@]3(CC[C@H]4[C@@]([C@H]3C1)(C)CCc1c4cco1)C[C@@]2(CO)O</chem>
InChI	DNJVYWXIDISQRD-HWUKTEKMSA-N
InChIKey	1S/C20H28O3/c1-18-7-5-16-14(6-9-23-16)15(18)4-8-19-10-13(2-3-17(18)19)20(22,11-19)12-21/h6,9,13,15,17,21-22H,2-5,7-8,10-12H2,1H3/t13-,15-,17+,18-,19+,20+/m1/s1