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## Typical Product Specifications & Properties

# Caffeine Sodium Benzoate

CAS Number: : 8000-95-1

Specifications	Limits
Molecular weight	338.29
SMILES	<chem>c12c(n(c(n(c1=O)C)=O)C)ncn2C.c1(ccccc1)C(=O)[O-].[Na+]</chem>
InChI	JWBPVFVNISJVEM-UHFFFAOYSA-M
InChIKey	1S/C8H10N4O2.C7H6O2.Na/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2;8-7(9)6-4-2-1-3-5-6;/h4H,1-3H3;1-5H,(H,8,9);/q;:+1/p-1



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