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## Typical Product Specifications & Properties

# Brucine sulfate heptahydrate

CAS Number: : 5787-00-8

Specifications	Limits
Molecular weight	1,013.12
SMILES	<chem>O.O.O.O.O.O.O.COc1cc2N3[C@H]4[C@@H]5[C@H](CC3=O)OCC=C6CN7CC[C@]4([C@@H]7C[C@H]56)c2cc1OC(Cc%10=O)OCC=C%13CN%14CC[C@]%11([C@@H]%14C[C@f</chem>
InChI	PPJIVFYMRNHHTJ-JYGVWXPPSA-N
InChIKey	1S/2C23H26N2O4.H2O4S.7H2O/c2*1-27-16-8-14-15(9-17(16)28-23(14,22(21)25)4-5-24(19)11-12(13)3-6-29-18;1-5(2,3)4;;;;;;;;/h2*(H2,1,2,3,4);7*1H2/t2*13-,18-,19-,21-,22-,23+;;;;;;;;/m00.....



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