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Typical Product Specifications & Properties

Sodium dehydrocholate

CAS Number: : 145-41-5

| Specifications | Limits |
|------------------|---|
| Molecular weight | 424.51 |
| SMILES | <chem>[C@H]12[C@H]3[C@@]([C@H](CC3)[C@@H](CCC(=O)[O-])C)(C(=O)C[C@@H]1[C@@]1([C@H](CC2=O)CC(=O)CC1)C)C.[Na+]</chem> |
| InChI | FKJIJBSJQSMPTI-CAOXKPNISA-M |
| InChIKey | 1S/C24H34O5.Na/c1-13(4-7-21(28)29)16-5-6-17-22-18(12-20(27)24(16,17)3)23(2)9-8-15(25)10-14(23)11-19(22)26;/h13-14,16-18,22H,4-12H2,1-3H3,(H,28,29);/q;+1/p-1/t13-,14+,16-,17+,18+,22+,23+,24-;/m1./s1 |



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