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Typical Product Specifications & Properties

Chenodeoxycholic acid

CAS Number: : 474-25-9

Specifications	Limits
Molecular weight	392.57
EINECS	207-481-8
SMILES	<chem>C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
InChI	RUDATBOHQWOJDD-BSWAIDMHSA-N
InChIKey	1S/C24H40O4/c1-14(4-7-21(27)28)17-5-6-18-22-19(9-11-24(17,18)3)23(2)10-8-16(25)12-15(23)13-20(22)26/h14-20,22,25-26H,4-13H2,1-3H3,(H,27,28)/t14-,15+,16-,17-,18+,19+,20-,22+,23+,24-/m1/s1
Atmospheric OH Rate Constant	5.28E-11 cm ³ /molecule-sec
Water solubility	89.9 mg/L
Vapor Pressure	3.00E-13 mm Hg
Henry's Law Constant	1.41E-11 atm-m ³ /mole
log P (octanol-water)	4.15
Melting Point	119 ° C
Water solubility	PRACTICALLY INSOLUBLE



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Specifications	Limits
Alpha	12 ° (c=1, CHCl ₃)
Merck	13,2062
Solubility	PRACTICALLY INSOLUBLE
Storage Temperature	Refrigerator
Melting Point	165-167 °C



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