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## Typical Product Specifications & Properties

# Lithocholic acid

CAS Number: : 434-13-9

Specifications	Limits
Molecular weight	376.57
EINECS	207-099-1
SMILES	<chem>C1[C@@]2([C@H](CC[C@H]2[C@@H]2CC[C@H]3[C@@](CC[C@H](O)C3)(C)[C@@H]2C1)[C@@H](CCC(=O)O)C)C</chem>
InChI	1S/C24H40O3/c1-15(4-9-22(26)27)19-7-8-20-18-6-5-16-14-17(25)10-12-23(16,2)21(18)11-13-24(19,20)3/h15-21,25H,4-14H2,1-3H3,(H,26,27)/t15-,16-,17-,18+,19-,20+,21+,23+,24-/m0/s1
InChIKey	SMEROWZSTRWXGI-VKPXTEDRSA-N
Vapor Pressure	2.58E-11 mm Hg
Water solubility	0.377 mg/L
log P (octanol-water)	6.190
Henry's Law Constant	3.86E-10 atm-m <sup>3</sup> /mole
Atmospheric OH Rate Constant	4.38E-11 cm <sup>3</sup> /molecule-sec
Melting Point	186 &deg; C
Refractive Index	35.5 &deg; (C=1, EtOH)



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Specifications	Limits
Storage Temperature	Refrigerator
Form	Powder
Flash Point	9?
Merck	5545
Melting Point	183-188 &deg;C
Color	White to off-white
Flash Point	9?



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