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Typical Product Specifications & Properties

Ursolic Acid

CAS Number: : 77-52-1

Specifications	Limits
Molecular weight	456.70
EINECS	201-034-0
SMILES	<chem>C1[C@@]2([C@@H]3[C@@](CC[C@H]2C(C)([C@H](C1)O)C)([C@@]1(C(=CC3)[C@H]2[C@@](CC1)(CC[C@H]([C@H]2C)C)C(O)=O)C)C</chem>
InChI	WCGUUGGRBIKTOS-GPOJBZ KASA-N
InChIKey	1S/C30H48O3/c1-18-10-15-30(25(32)33)17-16-28(6)20(24(30)19(18)2)8-9-22-27(5)13-12-23(31)26(3,4)21(27)11-14-29(22,28)7/h8,18-19,21-24,31H,9-17H2,1-7H3,(H,32,33)/t18-,19+,21+,22-,23+,24+,27+,28-,29-,30+/m1/s1
Atmospheric OH Rate Constant	1.27E-10 cm ³ /molecule-sec
log P (octanol-water)	7.920
Melting Point	284 ° C
Color	White to off-white
Alpha	59 ° (c=0.3, pyridine)
Storage Temperature	2-8°C
Form	Crystalline Powder or Needles



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Specifications	Limits
Melting Point	292 °C (dec.)
Merck	9890
Water solubility	insoluble



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