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Typical Product Specifications & Properties

Aconitine

CAS Number: : 302-27-2

Specifications	Limits
Molecular weight	645.74
EINECS	206-121-7
InChI	1S/C34H47NO11/c1-7-35-15-31(16-41-3)20(37)13-21(42-4)33-19-14-32(40)28(45-30(39)18-11-9-8-10-12-18)22(19)34(46-17(2)36,27(38)29(32)44-6)23(26(33)35)24(43-5)25(31)33/h8-12,19-29,37-38,40H,7,13-16H2,1-6H3
InChIKey	XFSBVAOIAHNAPC-UHFFFAOYSA-N
Water solubility	310 mg/L
Vapor Pressure	1.38E-20 mm Hg
Atmospheric OH Rate Constant	1.84E-10 cm ³ /molecule-sec
Melting Point	204 ° C
Henry's Law Constant	4.53E-26 atm-m ³ /mole
log P (octanol-water)	0.130



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