

Basic properties

Input	salvin
Molar mass	332.44 g/mol
Exact mass	332.198759382 Da
Formula	C ₂₀ H ₂₈ O ₄
Composition	C (72.26%), H (8.49%), O (19.25%)
Lipinski's rule of five	✗

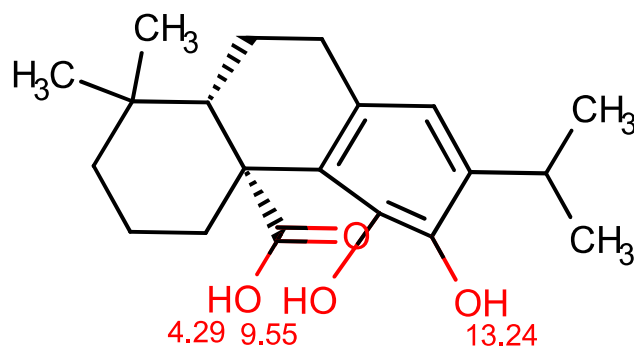
Structural properties

Atom count	52
Heavy atom count	24
Asymmetric atom count	2
Rotatable bond count	2
Ring count	3
Aromatic ring count	1
Hetero ring count	0
Hydrogen bond donor count	3
Hydrogen bond acceptor count	4
Formal charge	0
FSP3	0.65
Topological polar surface area	77.76 Å ²
Molar refractivity	93.41 cm ³ /mol
Polarizability	36.22 Å ³

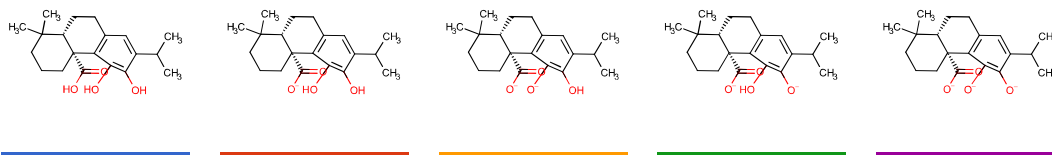
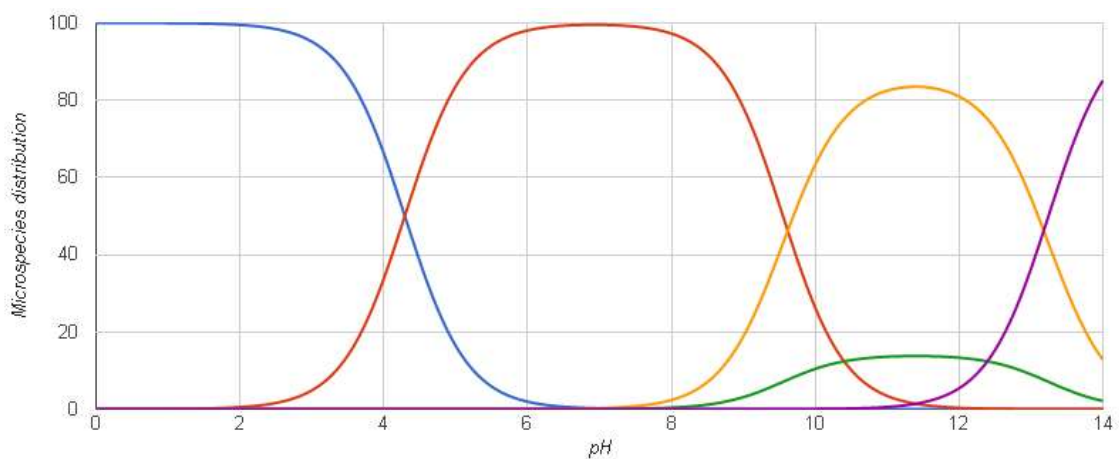
Names and identifiers

IUPAC name	(4aR,10aS)-5,6-dihydroxy-1,1-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-4a-carboxylic acid
Traditional name	salvin
Common names	carnosic acid; salvin
SMILES	<chem>CC(C)C1=CC2=C(C(O)=C1O)[C@]1(CCCC(C)(C)[C@@H]1CC2)C(O)=O</chem>
InChI	InChI=1S/C20H28O4/c1-11(2)13-10-12-6-7-14-19(3,4)8-5-9-20(14,18(23)24)15(12)17(22)16(13)21/h10-11,14,21-22H,5-9H2,1-4H3,(H,23,24)/t14-,20+/m0/s1
InChIKey	QRYRORQUOLYVBU-VBKZILBWSA-N
CAS	3650-09-7

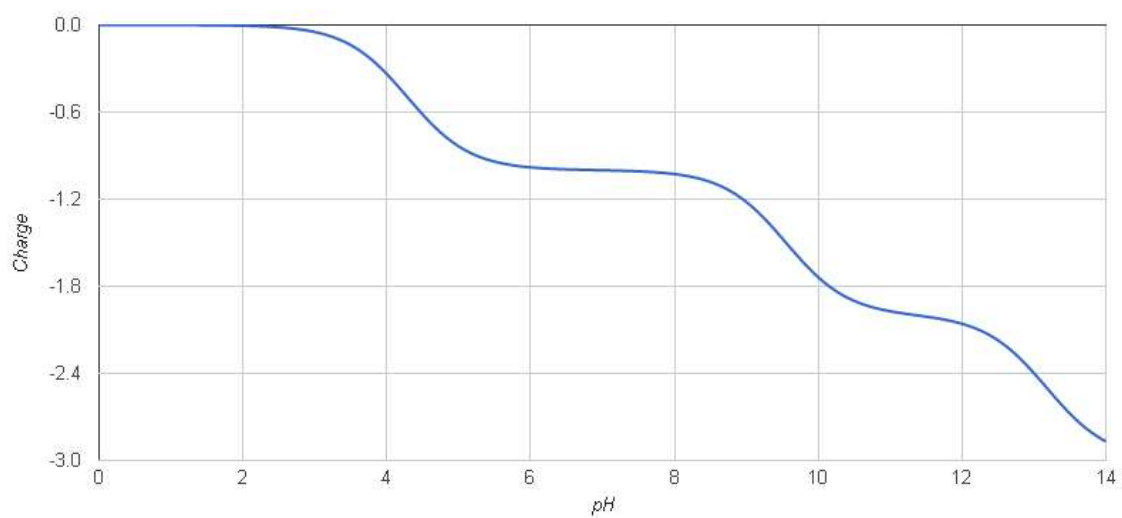
pKa



Strongest acidic pKa 4.29



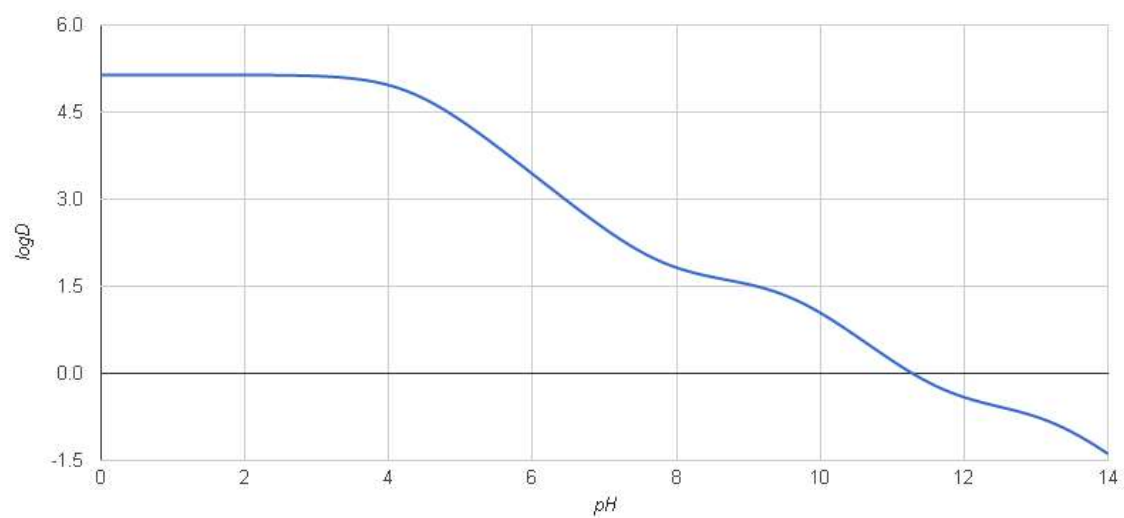
Isoelectric point



Isoelectric point: N/A

pH	Charge
1.7	-0.00
4.6	-0.67
6.5	-0.99
7.4	-1.01
8.0	-1.03

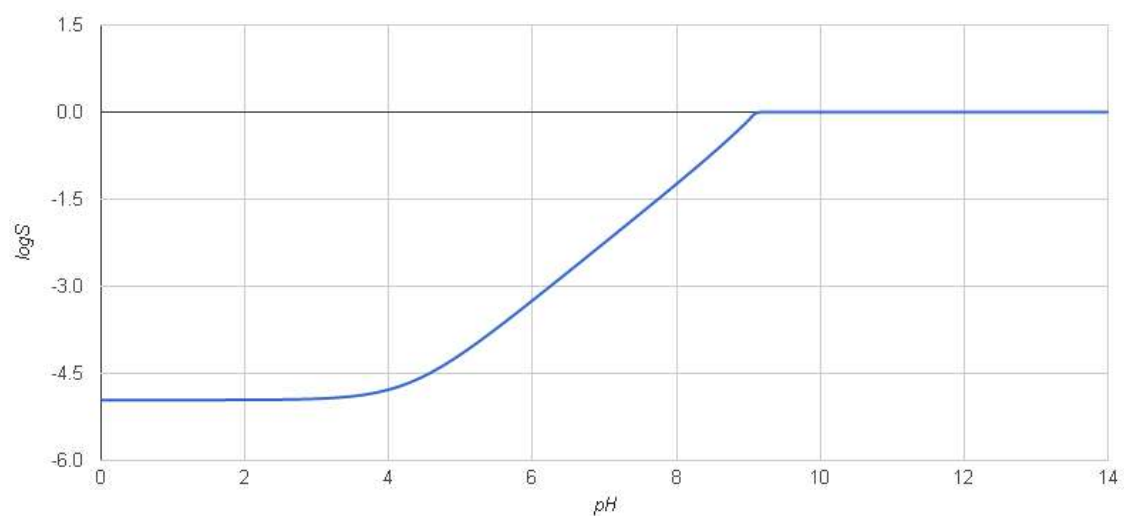
logP and logD



logP: 5.14

pH	logD
1.7	5.14
4.6	4.66
6.5	2.95
7.4	2.17
8.0	1.82

Solubility



Intrinsic solubility: -4.96

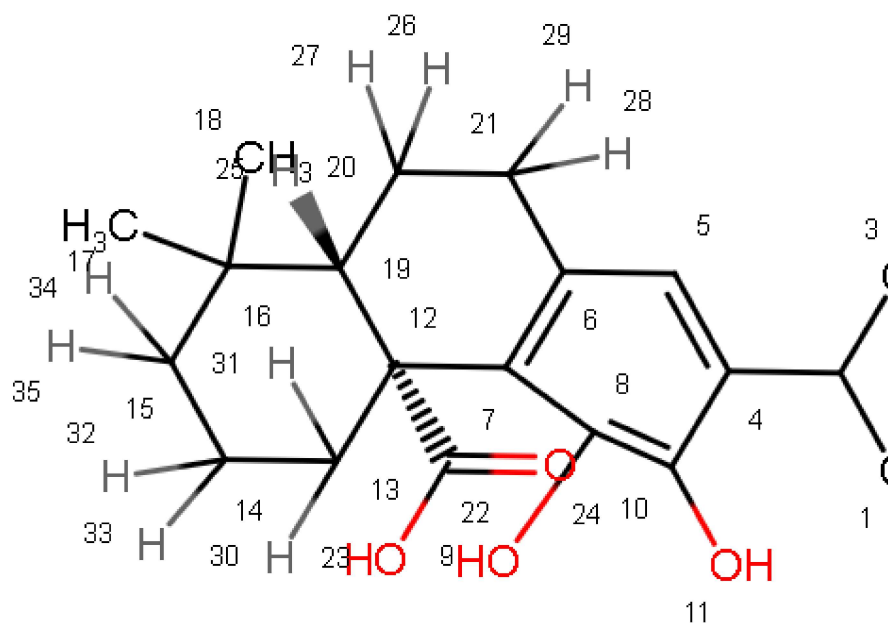
Solubility category: Low

pH	logS
1.7	-4.96
4.6	-4.48
6.5	-2.75
8.0	-1.24

Geometry

Van der Waals volume	326.50 Å ³
Van der Waals surface area	536.50 Å ²
Solvent accessible surface area	477.85 Å ²
Topological polar surface area	77.76 Å ²
Minimum projection area	49.78 Å ²
Maximum projection area	89.14 Å ²
Minimum projection radius	4.44 Å
Maximum projection radius	7.04 Å

H-NMR



Atoms	Shifts	Net intensity	Multiplet information	Quality
17,17,17,18,18,18	0.85 ppm	6	s	good
34	1.13 ppm	1	q	medium
1,1,1,3,3,3	1.19 ppm	6	d	good
26	1.36 ppm	1	o	medium
35	1.47 ppm	1	t	medium
32	1.51 ppm	1	n	medium
27	1.76 ppm	1	sx	medium
33	1.83 ppm	1	p	medium
30	2.04 ppm	1	q	medium
25	2.38 ppm	1	q	good
31	2.55 ppm	1	t	medium
28	2.68 ppm	1	o	good

29	2.76 ppm	1	sx	good
2	3.23 ppm	1	m	medium
5	6.31 ppm	1	q	medium
9	10.72 ppm	1	s	rough
11	10.72 ppm	1	s	rough
23	11.35 ppm	1	s	rough