

Valerenic acid

(*E*)-3-((4*S*,7*R*,7*aR*)-3,7-dimethyl-2,4,5,6,7,7*a*-hexahydro-1*H*-inden-4-yl)-2-methylacrylic acid

Chemical Formula: C<sub>15</sub>H<sub>22</sub>O<sub>2</sub>

Exact Mass: 234,16

Molecular Weight: 234,34

m/z: 234.16 (100.0%), 235.17 (16.6%), 236.17 (1.7%)

Elemental Analysis: C, 76.88; H, 9.46; O, 13.65

Boiling Point: 723,09 [K]

Melting Point: 446,75 [K]

Critical Temp: 817,65 [K]

Critical Pres: 20,59 [Bar]

Critical Vol: 755,5 [cm<sup>3</sup>/mol]

Gibbs Energy: -108,63 [kJ/mol]

Log P: 3,21

MR: 69,8 [cm<sup>3</sup>/mol]

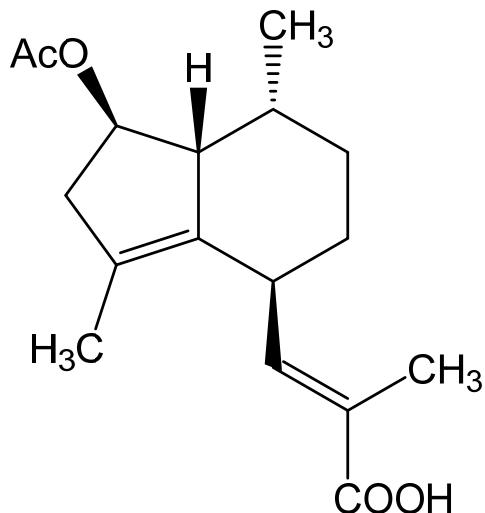
Henry's Law: 3,93

Heat of Form: -454,15 [kJ/mol]

tPSA: 37.3

CLogP: 4.737

CMR: 6.9936



Acetoxyvalerenic acid

(*E*)-3-((1*R*,4*S*,7*R*,7*aR*)-1-acetoxy-3,7-dimethyl-2,4,5,6,7,7*a*-hexahydro-1*H*-inden-4-yl)-2-methylacrylic acid

Chemical Formula: C<sub>17</sub>H<sub>24</sub>O<sub>4</sub>

Exact Mass: 292,17

Molecular Weight: 292,38

m/z: 292.17 (100.0%), 293.17 (18.8%), 294.17 (2.4%)

Elemental Analysis: C, 69.84; H, 8.27; O, 21.89

Boiling Point: 822,4 [K]

Melting Point: 507,38 [K]

Critical Temp: 849,4 [K]

Critical Pres: 17,02 [Bar]

Critical Vol: 892,5 [cm<sup>3</sup>/mol]

Gibbs Energy: -409,87 [kJ/mol]

Log P: 2,28

MR: 80,61 [cm<sup>3</sup>/mol]

Henry's Law: 6,55

Heat of Form: -833,05 [kJ/mol]

tPSA: 63.6

CLogP: 3.596

CMR: 8.11