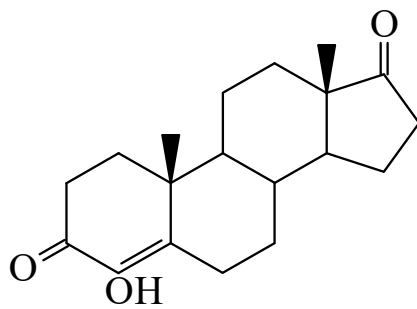




>>Entry Name: 4-Hydroxyandrost-4-ene-3,17-dione, 9CI  
Synonym(s): Formestane, BAN, INN. Lentaron. CGP 32349



CAS Registry Number: 566-48-3

Molecular Formula: C<sub>19</sub>H<sub>26</sub>O<sub>3</sub>  
Molecular Weight: 302.413  
Accurate Mass: 302.188195  
Percentage Composition: C 75.46%; H 8.67%; O 15.87%

Use/Importance: Aromatase inhibitor; antineoplastic agent. Used in chemotherapy of estrogen-sensitive breast cancer

Physical Description: Needles (EtOAc/petrol)

Development Status: Launched 1993 (UK)

Melting Point: Mp 205-206°

Optical Rotation: [ $\alpha$ ]<sub>D</sub><sup>20</sup>+181 (c, 7.7 in CHCl<sub>3</sub>)

Calculated Log P Data: Log P 2.74 (uncertain value) (calc)

Sigma: A5791

>>Derivative: Ac

CAS Registry Number: 61630-32-8  
Molecular Formula: C<sub>21</sub>H<sub>28</sub>O<sub>4</sub>  
Molecular Weight: 344.45  
Accurate Mass: 344.19876  
Percentage Composition: C 73.23%; H 8.19%; O 18.58%  
Physical Description: Cryst. (EtOAc/petrol)  
Melting Point: Mp 184°

Sigma: A9295

>>Derivative: Me ether

Synonym(s): 4-Methoxyandrost-4-ene-3,17-dione

CAS Registry Number: 20986-46-3

Molecular Formula: C<sub>20</sub>H<sub>28</sub>O<sub>3</sub>  
Molecular Weight: 316.439  
Accurate Mass: 316.203845  
Percentage Composition: C 75.91%; H 8.92%; O 15.17%  
Physical Description: Cryst. (Et<sub>2</sub>O)  
Melting Point: Mp 136-138°  
Optical Rotation: [ $\alpha$ ]<sub>D</sub><sup>20</sup>+177 (c, 7.6 in CHCl<sub>3</sub>)  
Sigma: A2542

#### References:

- Burnett, R.D. *et al.*, *J.C.S. Perkin 1*, 1973, 1830, (*synth, uv, ir, pmr*)  
Jennings, B.H. *et al.*, *Steroids*, 1978, **31**, 49, (*synth, uv, ir, pmr*)  
Griffin, J.F. *et al.*, *Acta Cryst. B*, 1980, **36**, 201, (*cryst struct*)  
Mann, J. *et al.*, *J.C.S. Perkin 1*, 1983, 2681, (*synth, ir, pmr, cmr*)  
Brodie, A.M.H. *et al.*, *Steroids*, 1987, **50**, 89, (*rev*)  
Kirk, D.N. *et al.*, *J.C.S. Perkin 2*, 1990, 1567, (*pmr*)  
Ciattini, P.G. *et al.*, *Synth. Commun.*, 1992, **22**, 1949, (*synth*)  
Wiseman, L.R., *Drugs*, 1993, **45**, 66, (*rev*)  
*Martindale, The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 482  
Dowsett, M. *et al.*, *Breast Cancer Res. Treat.*, 1994, **30**, 81, (*rev*)  
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HJB200