

Finasteride

Other names:

4-Azaandrost-1-ene-17-carboxamide, N-(1,1-dimethylethyl)-3-oxo-,
(5«alpha»,17«beta»)-
N-tert-Butyl-3-oxo-4-aza-5«alpha»-androst-1-ene-17«beta»-carboxamide
Chibro-Proscar
Finastid
MK-906
Propecia
Proscar
Prostide
Finpecia

Inchi: (5«alpha»,17«beta»)-N-(1,1-dimethylethyl)-3-oxo-4-azaandrost-1-ene-17-carboxamide
(Finasteride)
InchiKey: DBEPLOCGEIEOCV-UHFFFAOYSA-N
Formula: C₂₃H₃₆N₂O₂
SMILES: CC(C)(C)NC(=O)C1CCC2C3CCC4NC(=O)C=CC4(C)C3CCC12C
Mol. weight [g/mol]: 372.54
CAS: 98319-26-7

Physical Properties

Property code	Value	Unit	Source
gf	249.56	kJ/mol	Joback Method
hf	-398.16	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	87.26	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	3.814		Crippen Method
mcvol	310.290	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
tb	976.76	K	Joback Method
tc	1229.98	K	Joback Method
tf	717.23	K	Joback Method
vc	1.165	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.06	J/mol×K	976.76	Joback Method
cpg	1208.67	J/mol×K	1018.96	Joback Method
cpg	1240.19	J/mol×K	1061.17	Joback Method
cpg	1273.04	J/mol×K	1103.37	Joback Method
cpg	1307.66	J/mol×K	1145.57	Joback Method
cpg	1344.47	J/mol×K	1187.78	Joback Method
cpg	1383.92	J/mol×K	1229.98	Joback Method
hsubt	143.70	kJ/mol	475.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98319267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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