Methenolone

Other names: Androst-1-en-3-one, 17-hydroxy-1-methyl-, (5«alpha»,17«beta»)-
5«alpha»-Androst-1-en-3-one, 17«beta»-hydroxy-1-methyl-
Metenolone
Methenolon
17«beta»-Hydroxy-1-methyl-5«alpha»-androst-1-en-3-one
Inchi: InChI=1S/C20H30O2/c1-12-10-14(21)11-13-4-5-15-16-6-7-18(22)19(16,2)9-8-17(15)20(1
InchiKey: ANJQEDFWRSLVBR-IVKNRJJZSA-N
Formula: C20H30O2
SMILES: CC1=CC(=O)CC2CCC3C4CCC(O)C4(C)CCC3C12C
Mol. weight [g/mol]: 302.45
CAS: 153-00-4

Physical Properties

Property code	Value	Unit	Source
gf	26.83	kJ/mol	Joback Method
hf	-469.89	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.125		Crippen Method
mcvol	252.360	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2854.90		NIST Webbook
rinpol	2854.90		NIST Webbook
tb	855.92	K	Joback Method
tc	1089.09	K	Joback Method
tf	546.72	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.58	J/mol×K	855.92	Joback Method
cpg	929.32	J/mol×K	894.78	Joback Method

cpg	954.04	J/mol×K	933.64	Joback Method
cpg	979.06	J/mol×K	972.51	Joback Method
cpg	1004.66	J/mol×K	1011.37	Joback Method
cpg	1031.16	J/mol×K	1050.23	Joback Method
cpg	1058.86	J/mol×K	1089.09	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C153004&Units=SI

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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume