17-epi-Methandienone

Inchi: InChI=1S/C20H28O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1
InchiKey: XWALNWXLMVGSFR-BROHZWGRSA-N
Formula: C20H28O2
SMILES: CC12C=CC(=O)C=C1CCC1C2CCC2(C)C1CCC2(C)O
Mol. weight [g/mol]: 300.44

Physical Properties

Property code	Value	Unit	Source
gf	59.01	kJ/mol	Joback Method
hf	-376.53	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.045		Crippen Method
mcvol	248.060	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2724.00		NIST Webbook
tb	859.99	K	Joback Method
tc	1101.34	K	Joback Method
tf	575.62	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.37	J/mol×K	859.99	Joback Method
cpg	895.67	J/mol×K	900.21	Joback Method
cpg	923.03	J/mol×K	940.44	Joback Method
cpg	951.90	J/mol×K	980.66	Joback Method
cpg	982.76	J/mol×K	1020.89	Joback Method
cpg	1016.08	J/mol×K	1061.11	Joback Method
cpg	1052.32	J/mol×K	1101.34	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=R257806&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

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