

17-epi-Methyltestosterone

Inchi: InChI=1S/C20H30O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(21)
InchiKey: GCKMFJBGXUYNAG-BROHZWGRSA-N
Formula: C20H30O2
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CCC2(C)O
Mol. weight [g/mol]: 302.45

Physical Properties

Property code	Value	Unit	Source
gf	29.05	kJ/mol	Joback Method
hf	-434.31	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.269		Crippen Method
mvol	252.360	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rmpol	2685.00		NIST Webbook
tb	860.83	K	Joback Method
tc	1100.51	K	Joback Method
tf	574.86	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.24	J/mol×K	860.83	Joback Method
cpg	925.32	J/mol×K	900.78	Joback Method
cpg	953.37	J/mol×K	940.72	Joback Method
cpg	982.85	J/mol×K	980.67	Joback Method
cpg	1014.21	J/mol×K	1020.62	Joback Method
cpg	1047.90	J/mol×K	1060.56	Joback Method
cpg	1084.38	J/mol×K	1100.51	Joback Method

Sources

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=R257866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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