

Spiro[cyclopropan-1,6'-testosterone]

Inchi:	InChI=1S/C21H30O2/c1-19-7-5-13(22)11-17(19)21(9-10-21)12-14-15-3-4-18(23)20(15,2
InchiKey:	IFIMOKPOZBFPSW-UHFFFAOYSA-N
Formula:	C21H30O2
SMILES:	CC12CCC(=O)C=C1C1(CC1)CC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]:	314.46
CAS:	5083-34-1

Physical Properties

Property code	Value	Unit	Source
gf	110.32	kJ/mol	Joback Method
hf	-375.99	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.269		Crippen Method
mcvol	255.590	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
tb	886.18	K	Joback Method
tc	1128.66	K	Joback Method
tf	607.59	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.81	J/molxK	886.18	Joback Method
cpg	970.65	J/molxK	926.59	Joback Method
cpg	1001.02	J/molxK	967.01	Joback Method
cpg	1033.44	J/molxK	1007.42	Joback Method
cpg	1068.44	J/molxK	1047.84	Joback Method
cpg	1106.55	J/molxK	1088.25	Joback Method
cpg	1148.29	J/molxK	1128.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5083341&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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