

5-Androstene, 4,4-dimethyl-

Other names:	4,4,10,13-Tetramethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[1,2-b]pyridine
Inchi:	4,4-dimethyl-13«alpha»-androst-5-ene
InchiKey:	INCHI=1S/C21H34/c1-19(2)11-6-13-21(4)17-10-14-20(3)12-5-7-16(20)15(17)8-9-18(19)2
Formula:	C21H34
SMILES:	CC1(C)CCCC2(C)C1=CCC1C3CCCC3(C)CCC12
Mol. weight [g/mol]:	286.49

Physical Properties

Property code	Value	Unit	Source
gf	296.88	kJ/mol	Joback Method
hf	-165.02	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.366		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2219.35		NIST Webbook
rinpol	2219.35		NIST Webbook
tb	723.71	K	Joback Method
tc	968.95	K	Joback Method
tf	457.09	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.00	J/mol×K	723.71	Joback Method
cpg	861.71	J/mol×K	764.58	Joback Method
cpg	889.81	J/mol×K	805.46	Joback Method
cpg	917.82	J/mol×K	846.33	Joback Method
cpg	946.28	J/mol×K	887.21	Joback Method
cpg	975.73	J/mol×K	928.08	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=U194154&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
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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