

Androstan-17-one, (5«alpha»)-

Other names:	17-Oxo-5«alpha»-androstane 17-Oxo-5Â«alphaÂ»-androstane 5«alpha»-Androstan-17-one 5Â«alphaÂ»-Androstan-17-one androstane-17-one
Inchi:	InChI=1S/C19H30O/c1-18-11-4-3-5-13(18)6-7-14-15-8-9-17(20)19(15,2)12-10-16(14)18/
InchiKey:	YJDYCVLVYZDESB-CBXRHLNTSA-N
Formula:	C19H30O
SMILES:	CC12CCC3C(CCC4CCCCC43C)C1CCC2=O
Mol. weight [g/mol]:	274.44
CAS:	963-74-6

Physical Properties

Property code	Value	Unit	Source
gf	142.61	kJ/mol	Joback Method
hf	-322.99	kJ/mol	Joback Method
hfus	16.06	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-6.70		Aqueous Solubility Prediction Method
logp	4.988		Crippen Method
mvol	236.700	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
tb	741.39	K	Joback Method
tc	995.68	K	Joback Method
tf	393.00 ± 3.00	K	NIST Webbook
vc	0.888	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.31	J/mol×K	741.39	Joback Method
cpg	817.52	J/mol×K	783.77	Joback Method
cpg	844.73	J/mol×K	826.15	Joback Method

cpg	871.34	J/mol×K	868.54	Joback Method
cpg	897.76	J/mol×K	910.92	Joback Method
cpg	924.41	J/mol×K	953.30	Joback Method
cpg	951.68	J/mol×K	995.68	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C963746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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