

Androstane

Other names:	1H-Cyclopenta[a]phenanthrene, hexadecahydro-10,13-dimethyl-,
Inchi:	[8S-(8«alpha»,9«beta»,10«alpha»,13«alpha»,14«beta»)]-
InchiKey:	QZLYKIGBANMMBK-FSQANUGRSA-N
Formula:	C19H32
SMILES:	CC12CCCC1C1CCC3CCCCC3(C)C1CC2
Mol. weight [g/mol]:	260.46
CAS:	24887-75-0

Physical Properties

Property code	Value	Unit	Source
chs	-11740.00 ± 40.00	kJ/mol	NIST Webbook
gf	265.20	kJ/mol	Joback Method
hf	-185.29	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	55.48	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.809		Crippen Method
mcvol	235.130	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	673.57	K	Joback Method
tc	917.20	K	Joback Method
tf	397.37	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.85	J/molxK	673.57	Joback Method
cpg	770.96	J/molxK	714.17	Joback Method
cpg	798.54	J/molxK	754.78	Joback Method
cpg	824.99	J/molxK	795.38	Joback Method
cpg	850.70	J/molxK	835.99	Joback Method

cpg	876.09	J/mol×K	876.59	Joback Method
cpg	901.55	J/mol×K	917.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24887750&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

chs:	Standard solid enthalpy of combustion
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
mvol:	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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