

Androstane, (5«alpha»)-

Other names:	5«alpha»-Androstane Aetioallocholan 5alpha-Androstane Etioallocholane 5«alpha»-Androstan 5«alpha»,14«alpha»-Androstane NSC 49000 (5«alpha»).-androstane
Inchi:	InChI=1S/C19H32/c1-18-11-5-7-16(18)15-9-8-14-6-3-4-12-19(14,2)17(15)10-13-18/h14-
InchiKey:	QZLYKIGBANMMBK-DOQFWFFUSA-N
Formula:	C19H32
SMILES:	CC12CCCC1C1CCC3CCCCC3(C)C1CC2
Mol. weight [g/mol]:	260.46
CAS:	438-22-2

Physical Properties

Property code	Value	Unit	Source
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	2082.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2082.00		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/mol×K	673.57	Joback Method
cpg	770.96	J/mol×K	714.17	Joback Method
cpg	798.54	J/mol×K	754.78	Joback Method
cpg	824.99	J/mol×K	795.38	Joback Method
cpg	850.70	J/mol×K	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=C438222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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