Androstan-3-one, (5«alpha»)-

Other names: 5«alpha»-Androstan-3-one
Androstan-3-one
Inchi: InChI=1S/C19H30O/c1-18-9-3-4-16(18)15-6-5-13-12-14(20)7-11-19(13,2)17(15)8-10-18/
InchiKey: VMNRNUNYBVFVQI-OCUVBNDUSA-N
Formula: C19H30O
SMILES: CC12CCCC1C1CCC3CC(=O)CCC3(C)C1CC2
Mol. weight [g/mol]: 274.44
CAS: 1224-95-9

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	-5.18		Crippen Method
logp	4.988		Crippen Method
mcvol	236.700	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
tb	741.39	K	Joback Method
tc	995.68	K	Joback Method
tf	465.59	K	Joback Method
vc	0.888	m3/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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1224959&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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