Androst-5-en-4-one

Inchi: InChI=1S/C19H28O/c1-18-10-3-5-14(18)13-7-8-16-17(20)6-4-11-19(16,2)15(13)9-12-18/
InchiKey: MCYXUSLOLJKBAQ-TZNWLIJBSA-N
Formula: C19H28O
SMILES: CC12CCCC1C1CC=C3C(=O)CCCC3(C)C1CC2
Mol. weight [g/mol]: 272.43
CAS: 13583-72-7

Physical Properties

Property code	Value	Unit	Source
gf	170.65	kJ/mol	Joback Method
hf	-256.34	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	60.99	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.908		Crippen Method
mcvol	232.400	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2030.00		NIST Webbook
tb	750.20	K	Joback Method
tc	1007.29	K	Joback Method
tf	483.11	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.53	J/mol×K	750.20	Joback Method
cpg	788.17	J/mol×K	793.05	Joback Method
cpg	814.03	J/mol×K	835.90	Joback Method
cpg	839.54	J/mol×K	878.75	Joback Method
cpg	865.12	J/mol×K	921.60	Joback Method
cpg	891.20	J/mol×K	964.44	Joback Method
cpg	918.19	J/mol×K	1007.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13583727&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

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