Androsta-3,5-dien-17-one,3-ethoxy-

Inchi: InChI=1S/C21H30O2/c1-4-23-15-9-11-20(2)14(13-15)5-6-16-17-7-8-19(22)21(17,3)12-10
InchiKey: PAOWPNQOTVTCAF-UHFFFAOYSA-N
Formula: C21H30O2
SMILES: CCOC1=CC2=CCC3C4CCC(=O)C4(C)CCC3C2(C)CC1
Mol. weight [g/mol]: 314.46
CAS: 972-46-3

Physical Properties

Property code	Value	Unit	Source
gf	102.82	kJ/mol	Joback Method
hf	-383.53	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.049		Crippen Method
mcvol	262.150	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
tb	822.52	K	Joback Method
tc	1068.06	K	Joback Method
tf	541.16	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.76	J/mol×K	822.52	Joback Method
cpg	913.80	J/mol×K	863.44	Joback Method
cpg	939.59	J/mol×K	904.37	Joback Method
cpg	965.48	J/mol×K	945.29	Joback Method
cpg	991.82	J/mol×K	986.21	Joback Method
cpg	1018.95	J/mol×K	1027.14	Joback Method
cpg	1047.22	J/mol×K	1068.06	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=C972463&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume