3-Oxa-a-nor-5alpha-androstane-2-one, 5,17beta-dihydroxy-

Inchi: InChI=1S/C17H26O4/c1-15-7-6-12-10(11(15)3-4-13(15)18)5-8-17(20)16(12,2)9-14(19)21

InchiKey: WAJSBKRXXSZNLG-UHFFFAOYSA-N

Formula: C17H26O4

SMILES: CC12CCC3C(CCC4(O)OC(=O)CC34C)C1CCC2O

Mol. weight [g/mol]: 294.39

CAS: 3656-95-9

Physical Properties

Property code	Value	Unit	Source
gf	-235.09	kJ/mol	Joback Method
hf	-717.11	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.225		Crippen Method
mcvol	226.130	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	898.24	K	Joback Method
tc	1125.37	K	Joback Method
tf	614.44	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.72	J/mol×K	898.24	Joback Method
cpg	875.42	J/mol×K	936.09	Joback Method
cpg	901.48	J/mol×K	973.95	Joback Method
cpg	929.28	J/mol×K	1011.80	Joback Method
cpg	959.19	J/mol×K	1049.66	Joback Method
cpg	991.60	J/mol×K	1087.51	Joback Method
cpg	1026.89	J/mol×K	1125.37	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=C3656959&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