Androsta-5,9(11)-dien-3-one, 17beta-acetoxy-4-oxa-

Inchi: InChI=1S/C20H26O4/c1-12(21)23-16-7-5-14-13-4-6-17-20(3,11-9-18(22)24-17)15(13)8-1

InchiKey: MAULLEFJDUURPT-UHFFFAOYSA-N

Formula: C20H26O4

SMILES: CC(=O)OC1CCC2C3CC=C4OC(=O)CCC4(C)C3=CCC12C

Mol. weight [g/mol]: 330.42

CAS: 2455-42-7

Physical Properties

Property code	Value	Unit	Source
gf	-120.64	kJ/mol	Joback Method
hf	-607.47	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.912		Crippen Method
mcvol	255.500	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
tb	880.46	K	Joback Method
tc	1131.82	K	Joback Method
tf	606.39	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.40	J/mol×K	880.46	Joback Method
cpg	911.06	J/mol×K	922.35	Joback Method
cpg	936.01	J/mol×K	964.25	Joback Method
cpg	961.60	J/mol×K	1006.14	Joback Method
cpg	988.20	J/mol×K	1048.03	Joback Method
cpg	1016.15	J/mol×K	1089.92	Joback Method
cpg	1045.82	J/mol×K	1131.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2455427&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume