Androstane-3,11-dione, (5beta), 17beta-hydroxy-17alpha-methyl-

Inchi: InChI=1S/C20H30O3/c1-18-8-6-13(21)10-12(18)4-5-14-15-7-9-20(3,23)19(15,2)11-16(22

InchiKey: SLGYIGUMKJYZLP-UHFFFAOYSA-N

Formula: C20H30O3

SMILES: CC12CCC(=O)CC1CCC1C2C(=O)CC2(C)C1CCC2(C)O

Mol. weight [g/mol]: 318.45

CAS: 59962-27-5

Physical Properties

Property code	Value	Unit	Source
gf	-121.58	kJ/mol	Joback Method
hf	-638.66	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.528		Crippen Method
mcvol	258.230	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
tb	919.84	K	Joback Method
tc	1166.40	K	Joback Method
tf	625.56	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.96	J/mol×K	919.84	Joback Method
cpg	1008.06	J/mol×K	960.93	Joback Method
cpg	1039.48	J/mol×K	1002.03	Joback Method
cpg	1072.66	J/mol×K	1043.12	Joback Method
cpg	1108.05	J/mol×K	1084.21	Joback Method
cpg	1146.10	J/mol×K	1125.31	Joback Method
cpg	1187.25	J/mol×K	1166.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59962275&Units=SI

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