Androstane, 3,17-dione, (5alpha), 2alpha-methyl-

Inchi: InChI=1S/C20H30O2/c1-12-11-20(3)13(10-17(12)21)4-5-14-15-6-7-18(22)19(15,2)9-8-16

InchiKey: RVSSFXUENQNQJK-UHFFFAOYSA-N

Formula: C20H30O2

SMILES: CC1CC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)CC1=O

Mol. weight [g/mol]: 302.45

CAS: 5470-27-9

Physical Properties

Property code	Value	Unit	Source
gf	20.73	kJ/mol	Joback Method
hf	-501.67	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	65.89	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.413		Crippen Method
mcvol	252.360	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
tb	827.42	K	Joback Method
tc	1085.78	K	Joback Method
tf	540.84	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.92	J/mol×K	827.42	Joback Method
cpg	927.52	J/mol×K	870.48	Joback Method
cpg	955.60	J/mol×K	913.54	Joback Method
cpg	983.53	J/mol×K	956.60	Joback Method
cpg	1011.67	J/mol×K	999.66	Joback Method
cpg	1040.38	J/mol×K	1042.72	Joback Method
cpg	1070.03	J/mol×K	1085.78	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=C5470279&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