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

Other names: 5«beta»-Androstane-11,17-dione, 3«alpha»-hydroxy-
Ba 2684
Etiocholanol-11-one
11-Ketoetiocholanolone
11-Oxoaetiocholanolone
11-Oxoetiocholanolone
3«alpha»-Hydroxy-11,17-dioxo-5«beta»-androstane
3«alpha»-Hydroxy-5«beta»-androstane-11,17-dione
5«beta»-Androstan-3«alpha»-ol-11,17-dione
3-Hydroxyandrostane-11,17-dione, (3«alpha»,5«beta»)-
3alpha-hydroxy-5beta-Androstane-11,17-dione
NSC 53896

Inchi: InChI=1S/C19H28O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17

InchiKey: IUNYGQONJQTULL-UXMFXKFTSA-N

Formula: C19H28O3

SMILES: CC12CC(=O)C3C(CCC4CC(O)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 304.42

CAS: 739-27-5

Physical Properties

Property code	Value	Unit	Source
gf	-124.51	kJ/mol	Joback Method
hf	-633.26	kJ/mol	Joback Method
hfus	20.73	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.138		Crippen Method
mcvol	244.140	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
tb	896.72	K	Joback Method
tc	1140.10	K	Joback Method
tf	590.39	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.93	J/mol×K	896.72	Joback Method
cpg	939.35	J/mol×K	937.28	Joback Method
cpg	964.88	J/mol×K	977.85	Joback Method
cpg	990.81	J/mol×K	1018.41	Joback Method
cpg	1017.44	J/mol×K	1058.97	Joback Method
cpg	1045.09	J/mol×K	1099.53	Joback Method
cpg	1074.05	J/mol×K	1140.10	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C739275&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

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