5Alpha-androsta-1-ene-3,11,17-trione

Inchi: InChI=1S/C19H24O3/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: NYLSQMMWVJMFFO-UHFFFAOYSA-N

Formula: C19H24O3

SMILES: CC12CC(=O)C3C(CCC4CC(=O)C=CC43C)C1CCC2=O

Mol. weight [g/mol]: 300.39

CAS: 7339-06-2

Physical Properties

Property code	Value	Unit	Source
gf	-72.61	kJ/mol	Joback Method
hf	-540.61	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	68.51	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.122		Crippen Method
mcvol	235.540	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
tb	876.19	K	Joback Method
tc	1150.84	K	Joback Method
tf	602.79	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.97	J/mol×K	876.19	Joback Method
cpg	875.15	J/mol×K	921.97	Joback Method
cpg	902.23	J/mol×K	967.74	Joback Method
cpg	929.61	J/mol×K	1013.52	Joback Method
cpg	957.65	J/mol×K	1059.29	Joback Method
cpg	986.76	J/mol×K	1105.07	Joback Method
cpg	1017.31	J/mol×K	1150.84	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=C7339062&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