Androsta-1,4-diene-3,11,17-trione

Other names: 1,4-Androstadiene-3,11,17-trione
Inchi: InChI=1S/C19H22O3/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: RZACPWSZIQKVDY-GFPCFBFFSA-N
Formula: C19H22O3
SMILES: CC12C=CC(=O)C=C1CCC1C2C(=O)CC2(C)C(=O)CCC12
Mol. weight [g/mol]: 298.38
CAS: 7738-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-44.57	kJ/mol	Joback Method
hf	-473.96	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.042		Crippen Method
mcvol	231.240	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
tb	885.00	K	Joback Method
tc	1162.20	K	Joback Method
tf	620.31	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.88	J/mol×K	885.00	Joback Method
cpg	841.05	J/mol×K	931.20	Joback Method
cpg	867.40	J/mol×K	977.40	Joback Method
cpg	894.32	J/mol×K	1023.60	Joback Method
cpg	922.22	J/mol×K	1069.80	Joback Method
cpg	951.49	J/mol×K	1116.00	Joback Method
cpg	982.54	J/mol×K	1162.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7738934&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