Canrenone

Other names: Pregna-4,6-diene-21-carboxylic acid, 17-hydroxy-3-oxo-, «gamma»-lactone, (17«alpha»)-

17«alpha»-Pregna-4,6-diene-21-carboxylic acid, 17-hydroxy-3-oxo-, «gamma»-lactone

Aldadiene

Canrenon

Phanurane

Spirolactone SC 14266

SC 9376

RP 11641

17«alpha»-(2-Carboxyethyl)-17«beta»-hydroxyandrosta-4,6-dien-3-one lactone

17-Hydroxy-3-oxo-17«alpha»-pregna-4,6-diene-21-carboxylic acid «gamma»-lactone

Spiro[17H-cyclopenta[a]phenanthrene-17,2'(5'H)-furan], pregna-4,6-diene-21-carboxylic acid deriv.

20-Spiroxa-4,6-diene-3,21-dione

11614 R.P.

17-Hydroxy-3-oxo-17«alpha»-pregna-4,6-diene-21-carboxylic acid lactone

NSC 261713

Inchi: InChI=1S/C22H28O3/c1-20-9-5-15(23)13-14(20)3-4-16-17(20)6-10-21(2)18(16)7-11-22(2

InchiKey: UJVLDDZCTMKXJK-UHFFFAOYSA-N

Formula: C22H28O3

SMILES: CC12CCC(=O)C=C1C=CC1C2CCC2(C)C1CCC21CCC(=O)O1

Mol. weight [g/mol]: 340.46

CAS: 976-71-6

Physical Properties

Property code	Value	Unit	Source
gf	60.32	kJ/mol	Joback Method
hf	-448.30	kJ/mol	Joback Method
hfus	22.04	kJ/mol	Joback Method
hvap	75.65	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.370		Crippen Method
mcvol	266.950	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
tb	924.02	K	Joback Method
tc	1202.24	K	Joback Method
tf	650.79	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.53	J/mol×K	924.02	Joback Method
cpg	1021.63	J/mol×K	970.39	Joback Method
cpg	1057.87	J/mol×K	1016.76	Joback Method
cpg	1096.96	J/mol×K	1063.13	Joback Method
cpg	1139.61	J/mol×K	1109.50	Joback Method
cpg	1186.52	J/mol×K	1155.87	Joback Method
cpg	1238.40	J/mol×K	1202.24	Joback Method

Sources

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=C976716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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