17«alpha»,21-Dihydroxypregn-4-en-3,20-dione, 17,21-anhydro (oxetanone)

Inchi: InChI=1S/C21H28O3/c1-19-8-5-14(22)11-13(19)3-4-15-16(19)6-9-20(2)17(15)7-10-21(20
InchiKey: SMVGGQBTFHTJLW-YUXGLXIYSA-N
Formula: C21H28O3
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CCC21OCC1=O
Mol. weight [g/mol]: 328.45

Physical Properties

Property code	Value	Unit	Source
gf	34.04	kJ/mol	Joback Method
hf	-479.28	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	72.96	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.856		Crippen Method
mcvol	257.160	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tb	897.71	K	Joback Method
tc	1172.36	K	Joback Method
tf	642.28	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.91	J/mol×K	897.71	Joback Method
cpg	979.53	J/mol×K	943.48	Joback Method
cpg	1013.99	J/mol×K	989.26	Joback Method
cpg	1050.96	J/mol×K	1035.03	Joback Method
cpg	1091.14	J/mol×K	1080.81	Joback Method
cpg	1135.23	J/mol×K	1126.58	Joback Method
cpg	1183.89	J/mol×K	1172.36	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=R525025&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume