A-norandrost-3(5)-en-2-one, 17-hydroxy-, cyclic ethylene acetal

Inchi: InChI=1S/C20H30O3/c1-18-8-7-16-14(15(18)5-6-17(18)21)4-3-13-11-20(12-19(13,16)2)2
InchiKey: WGOIRXCGJHBAPL-UHFFFAOYSA-N
Formula: C20H30O3
SMILES: CC12CC3(C=C1CCC1C2CCC2(C)C(O)CCC12)OCCO3
Mol. weight [g/mol]: 318.45
CAS: 2429-36-9

Physical Properties

Property code	Value	Unit	Source
gf	40.15	kJ/mol	Joback Method
hf	-487.81	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	83.12	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.663		Crippen Method
mcvol	251.670	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
tb	853.65	K	Joback Method
tc	1091.69	K	Joback Method
tf	577.72	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.98	J/mol×K	853.65	Joback Method
cpg	938.63	J/mol×K	893.32	Joback Method
cpg	966.43	J/mol×K	933.00	Joback Method
cpg	995.88	J/mol×K	972.67	Joback Method
cpg	1027.52	J/mol×K	1012.35	Joback Method
cpg	1061.86	J/mol×K	1052.02	Joback Method
cpg	1099.41	J/mol×K	1091.69	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=C2429369&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