A-norandrost-3(5)-en-2-one, 3,17-dihydroxy-

Inchi: InChI=1S/C18H26O3/c1-17-8-7-12-10(11(17)5-6-15(17)20)3-4-13-16(21)14(19)9-18(12,1
InchiKey: BCMRIYGWARNVDI-UHFFFAOYSA-N
Formula: C18H26O3
SMILES: CC12CC(=O)C(O)=C1CCC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]: 290.40
CAS: 1509-39-3

Physical Properties

Property code	Value	Unit	Source
gf	-116.65	kJ/mol	Joback Method
hf	-565.81	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	92.30	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.375		Crippen Method
mcvol	230.050	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
tb	907.72	K	Joback Method
tc	1131.90	K	Joback Method
tf	605.28	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.58	J/mol×K	907.72	Joback Method
cpg	867.57	J/mol×K	945.08	Joback Method
cpg	890.18	J/mol×K	982.45	Joback Method
cpg	913.69	J/mol×K	1019.81	Joback Method
cpg	938.38	J/mol×K	1057.17	Joback Method
cpg	964.52	J/mol×K	1094.53	Joback Method
cpg	992.38	J/mol×K	1131.90	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=C1509393&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