

Spiro(cyclopropane-1,6'-b-norandrost(4')en)-3'-one-17-b-hydroxy-17-methyl-

InChI:

InChI=1S/C21H30O2/c1-18-7-4-13(22)12-16(18)21(10-11-21)17-14(18)5-8-19(2)15(17)6

InchiKey:

MEJBPKQUIWLJSL-UHFFFAOYSA-N

Formula:

C21H30O2

SMILES:

CC12CCC(=O)C=C1C1(CC1)C1C2CCC2(C)C1CCC2(C)O

Mol. weight [g/mol]:

314.46

CAS:

17506-52-4

Physical Properties

Property code	Value	Unit	Source
gf	116.93	kJ/mol	Joback Method
hf	-354.59	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.269		Crippen Method
mcvol	255.590	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
tb	882.15	K	Joback Method
tc	1125.54	K	Joback Method
tf	635.01	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.64	J/molxK	882.15	Joback Method
cpg	965.81	J/molxK	922.72	Joback Method
cpg	999.55	J/molxK	963.28	Joback Method
cpg	1036.52	J/molxK	1003.85	Joback Method
cpg	1077.39	J/molxK	1044.41	Joback Method
cpg	1122.82	J/molxK	1084.98	Joback Method
cpg	1173.47	J/molxK	1125.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C17506524&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

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