

17-«beta»-Hydroxy-17-«alpha»-methyl-5-«beta»-a

Inchi:	InChI=1S/C20H30O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(
InchiKey:	JRNSSSJKIGAFCT-IEXXVWD TSA-N
Formula:	C20H30O2
SMILES:	CC12C=CC(=O)CC1CCC1C2CCC2(C)C1CCC2(C)O
Mol. weight [g/mol]:	302.45

Physical Properties

Property code	Value	Unit	Source
gf	30.97	kJ/mol	Joback Method
hf	-443.18	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	77.46	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.125		Crippen Method
mvol	252.360	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	2593.00		NIST Webbook
tb	851.18	K	Joback Method
tc	1090.22	K	Joback Method
tf	558.10	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.05	J/molxK	851.18	Joback Method
cpg	928.10	J/molxK	891.02	Joback Method
cpg	955.94	J/molxK	930.86	Joback Method
cpg	985.02	J/molxK	970.70	Joback Method
cpg	1015.79	J/molxK	1010.54	Joback Method
cpg	1048.70	J/molxK	1050.38	Joback Method
cpg	1084.19	J/molxK	1090.22	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=R257351&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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