

Pregna-5,16-dien-20-one, 3-hydroxy-, (3«beta»)-

Other names:

Pregna-5,16-dien-20-one, 3«beta»-hydroxy-
«delta»16-Pregnenolone
16-Dehydropregnenolone
16-Dehydropregmolone
Pregna-5,16-dienolone
5,16-Pregnadien-3«beta»-ol-20-one
5,16-Pregnadien-3beta-ol-20-one
3-«beta»-hydroxypregna-5,16-dien-20-one

Inchi: InChI=1S/C21H30O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2

InchiKey: YLFRRPUBVUAHSR-VJQWSGFBSA-N

Formula: C21H30O2

SMILES: CC(=O)C1=CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 314.46

CAS: 1162-53-4

Physical Properties

Property code	Value	Unit	Source
gf	56.96	kJ/mol	Joback Method
hf	-398.76	kJ/mol	Joback Method
hfus	29.09	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.435		Crippen Method
mcvol	262.150	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
tb	873.66	K	Joback Method
tc	1102.41	K	Joback Method
tf	557.22	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.24	J/molxK	873.66	Joback Method

cpg	940.91	J/mol×K	911.78	Joback Method
cpg	964.93	J/mol×K	949.91	Joback Method
cpg	989.63	J/mol×K	988.03	Joback Method
cpg	1015.33	J/mol×K	1026.16	Joback Method
cpg	1042.38	J/mol×K	1064.28	Joback Method
cpg	1071.08	J/mol×K	1102.41	Joback Method

Sources

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=C1162534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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