

PREGN-5-EN-20-ONE, 3-HYDROXY-

Other names:	5-Pregnene-3-ol-20-one
Inchi:	InChI=1S/C21H32O2/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:	ORNBQBCIOKFOEO-QXLQSZHOSA-N
Formula:	C21H32O2
SMILES:	CC(=O)[C@H]1CC[C@H]2[C@@H]3CC=C4CC(O)CC[C@]4(C)[C@H]3CC[C@]12C
Mol. weight [g/mol]:	316.48

Physical Properties

Property code	Value	Unit	Source
hfus	29.32	kJ/mol	Joback Method
hvap	119.85	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.31		Cheméo Relay (1.0)
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
tb	661.98	K	Cheméo Relay (1.0)
tf	449.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.54	J/mol×K	864.85	Joback Method
cpg	974.02	J/mol×K	902.61	Joback Method
cpg	998.64	J/mol×K	940.37	Joback Method
cpg	1023.72	J/mol×K	978.14	Joback Method
cpg	1049.57	J/mol×K	1015.90	Joback Method
cpg	1076.50	J/mol×K	1053.66	Joback Method
cpg	1104.85	J/mol×K	1091.42	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38372246&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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